



ESM TODAY 2015

12th Graduate Research Symposium

February 28, 2015

EES Bldg. 1st Floor Lobby

Department of
Engineering Science and Mechanics

Abstract Book

Keynote Speaker: Dr. Renata S. Engel

Dr. Renata S. Engel is Associate Vice Provost for Online Programs at The Pennsylvania State University. In that role, she has responsibility for the academic affairs of Penn State's World Campus, which encompasses the 120+ undergraduate, graduate online degree programs, minors and certificates and includes support for academic advising, faculty teaching online, and the development, piloting, and evaluation of online curricular innovations and enhancements. A member of the Penn State faculty since 1990, she is Professor of Engineering Design and Engineering Science and Mechanics, and served as the Associate Dean for Academic Programs in the College of Engineering from 2006-2014 and the Executive Director of the Schreyer Institute for Teaching Excellence at Penn State from 2000-2006.

Dr. Engel is a Fellow of the American Society for Engineering Education. She has held several leadership positions in that professional organization, including seven years on its Board of Directors, and President in 2010-2011. She currently serves as a delegate to the American Association for Engineering Societies (AAES).

Dr. Engel earned a BS (Honors '82) in Engineering Science from Penn State and a PhD '88 in Engineering Mechanics from the University of South Florida.

SCHEDULE

Time	Event		Duration
8:30 - 9:00 AM	Breakfast		30 min
9:00 - 9:15 AM	Introduction by Dr. Judith A. Todd		15 min
9:15 - 9:45 AM	Keynote Speech by Dr. Renata S. Engel		30 min
10:00 - 11:20 AM	4 Presentations	4 Presentations	80 min
11:20 - 11:30 AM	Break		10 min
11:30 - 12:50 PM	3 Presentations	4 Presentations	80 min
12:50 - 1:50 PM	Lunch and Poster Review		60 min
1:50 - 2:00 PM	Deliberation		10 min
2:00 PM	Awards Ceremony		15 min

PRESENTATION SCHEDULE

EES RM 114		EES RM 116	
Time	Presenter	Time	Presenter
10:00	Chandraprakash Chindam	10:00	Jeong Nyeon Kim
10:20	Baiyang Ren	10:20	Sema Erten
10:40	Jason Sheldon	10:40	Hwanjeong Cho
11:00	Abdon Pena-Francesch	11:00	Andrew Geronimo
Break		Break	
11:30	Stephen Swiontek	11:30	Alireza Ostadhossein
11:50	Gloria Choi	11:50	Justin Kauffman
12:10	Nicholas Labarbera	12:10	Huilong Huo
12:30	Nitesh Nama		

Poster presentations will be held in the EES 1st floor lobby from 12.50 pm to 1.50 pm

LIST OF JUDGES

Dr. Albert Segall
Dr. Akhlesh Lakhtakia
Dr. Sulin Zhang
Dr. Jonathan S. Pitt
Dr. Corina Drapaca

Dr. Michael Lanagan
Dr. Renata S. Engel
Dr. Bernhard Tittmann
Dr. Ivica Smid
Dr. Judith A. Todd

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ORAL PRESENTATIONS

MICROFIBER INCLINATION AND CRYSTALLINITY OF COLUMNAR THIN FILMS OF PARYLENE C

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Among the family of Xylylenes, called Parylenes, Parylene C has been of industrial interest as moisture-impermeable and electrical insulation coatings [1]. Recently, this material has been used for fabricating inhomogeneous thin films comprising periodically arranged microfibers (of columnar, chevronic and chiral morphologies) [2] which are explored for multiple functions including the growth of bioscaffolds [3]. Although the fabrication procedure for bulk and the microfibrinous thin films are established, a fundamental understanding of the material microstructure – amorphous and crystalline phases – and their dependence on deposition methods are not known. As a first step, here, we determine the dependence of microfiber inclination on deposition angle of columnar thin films (CTF) and determine the nature of crystallinity in these films and contrast this with a bulk film.

Silicon and brass substrates of dimensions $0.5 \times 0.5 \text{ in}^2$ are cleaned with standard cleaning procedure SC-1. The substrate configuration and the coordinate convention for deposition of columnar thin films are schematically shown in Fig. 1. CTFs of different microfiber inclinations (χ) are deposited with by varying the monomer vapor (χ_v) from 30° to 90° . A, a bulk film is also fabricated in the reduced capacity chamber. The deposition parameters of furnace 690°C , vaporizer 175°C , and vacuum 28 mTorr were the same for both kinds of depositions. The cross-sections of CTFs are imaged using a scanning electron microscope (SEM). A typical cross-sectional micrograph of a CTF is shown in Fig. 2a. The cross-section morphology of the CTF comprises parallel strands of microfibers placed 2-3 μm apart. The variation of the microfiber angle (χ) with deposition angle of the monomer vapor (χ_v) is shown in Fig. 2b. An increasing and intermittently constant kind of dependence of χ with χ_v is observed.

To explain the observed dependence of χ on

χ_v X-ray diffraction (XRD) experiments were performed. The reflection mode XRD patterns were collected on all brass samples in an Empyrean (PANalytical) theta-theta system using an automatic divergence slit. Operating at 45 kV and 40 mA, 2θ was varied from 5° to 70° . The crystal structure file for Parylene-C polymer was constructed and the plausible crystal planes are identified. A comparison of XRD patterns of CTFs with bulk film indicated the presence of the additional planes in the former, as shown in Fig. 3. Comparing the XRD patterns of CTFs, we observe that CTFs in the regime A and C (where χ is invariant with χ_v), see Fig. 2b, had a higher intensity than those of those belonging to the regimes B and D (where χ is linearly dependent on χ_v). A high intensity for regimes A and C confirms the preferred orientation of the monomers for those monomer vapor deposition angles. The crystallinity percentages, calculated by regression fit of XRD intensities to sum of 4 gaussian models, also revealed that regimes A and C had a higher percentage than B and D, thereby confirmation the preferred orientation for particular deposition angles. Geneva-gear mechanism was identified as a suitable theoretical model to convey the relation between χ and χ_v ; this same is shown in Fig. 2b, identified as ‘Equation (1)’.

The dependence of microfiber inclination on the deposition angle has been determined and a phenomenological model has been proposed for the same. We also identified the crystal planes and the crystallinity of CTFs and contrasted with a bulk film’s XRD signature. Therefore, these results would be useful in explaining the dependence of microstructure of chevron and chiral sculptured thin films on the monomer flux angle. The identified planes will also be helpful in explaining the mechanical and dielectric properties of morphologically different sculptured thin films [2] of Parylene C.

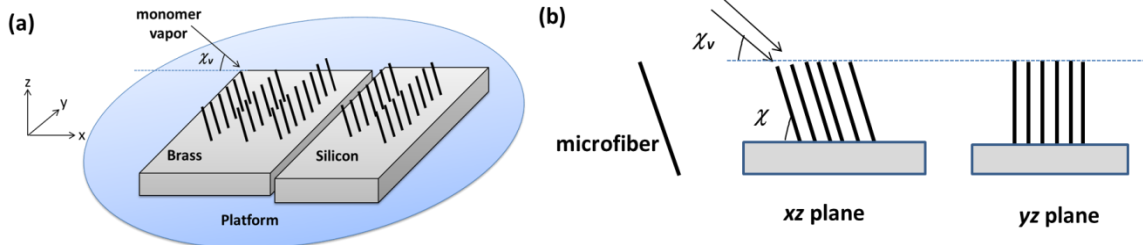


Figure 1: Schematic of the isometric view of a columnar film grown simultaneously on a brass wafer and silicon wafer mounted side by side on a rotatable platform, with χ_v as the angle between the collimated vapor and the wafer

plane. The wafer surface is designated as the xy plane, whereas the velocities of the reactive monomers lie wholly in the xz plane (b) Schematics of the plan views of the columnar film in the xz and yz planes.

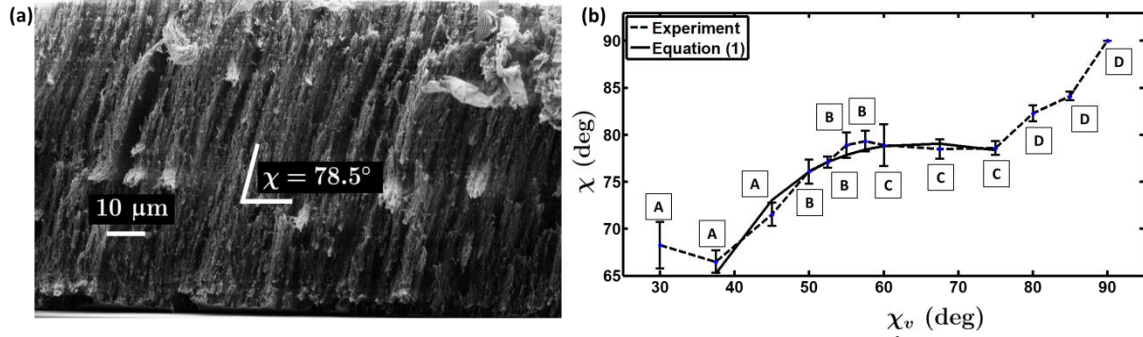


Figure 2: (a) Cross-sectional SEM image in the xz plane of the fabricated with $\chi_v = 57.5^\circ$. The microfiber inclination angle $\chi = 78.5^\circ$ for this sample. (b) Variation of χ with χ_v . The dashed line joins the means of five measured values of χ for every χ_v selected. The solid line represents Geneva gear model. Every CTF is classified as belonging to one of Groups A–D.

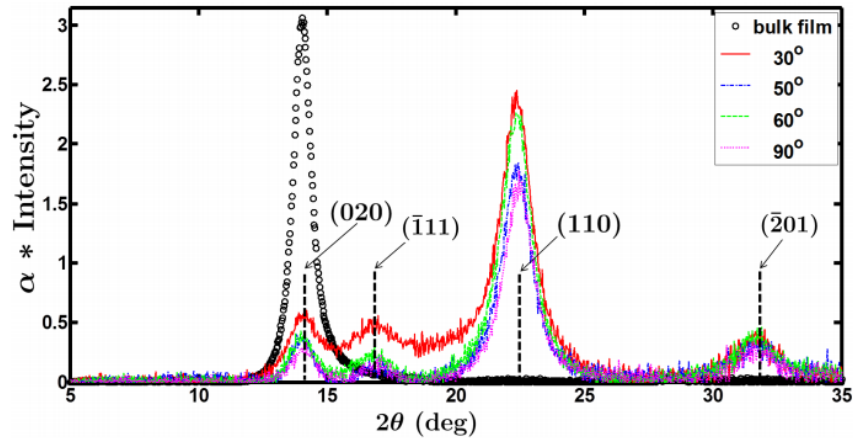


Figure 3: Comparison of XRD patterns of four different columnar μFTFS ($\chi_v \in \{30^\circ, 50^\circ, 60^\circ, 90^\circ\}$) and the bulk film. The normalization factor $\alpha = 5 \times 10^{-4}$ for all μFTFS but $\alpha = 10^{-4}$ for the bulk film. The Miller indices for the crystal plane for each peak are also provided.

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Electrical impedance matching network for ultrasonic phased array transducer and its effect on guided wave excitation

Baiyang Ren, Cliff J. Lissenden

Ultrasonic guided waves have been widely used in nondestructive evaluation (NDE) and structural health monitoring (SHM) because of their long propagation distance and good sensitivity to different defect types. However, in the field test, the damage detection technique could fail due to the changing operational conditions, e.g. temperature, loading and coupling condition, whose effects could easily overwhelm the defect induced change. To overcome this, using mode conversion as a damage indicator instead of amplitude and time of flight change has been proposed and tested by the author [1]. Also, phased array transducer for guided wave excitation in SHM is also designed to preferentially excite single guided wave mode [2].

Composite materials are widely used for aircrafts because they have high specific strength and stiffness. However, composite structures in aircraft are subject to different defects and need an online monitoring technique. Being able to reach inaccessible region and be sensitive to different defects make ultrasonic guided wave a promising tool. However, the resin matrix in composite materials is viscoelastic and usually causes severe attenuation to the propagating wave. Increasing the power of guided wave will enlarge the area covered by the transducer and enhance the signal to noise ratio. To increase the power delivered to the substrate, adding acoustic matching layers and electrical impedance matching networks are two popular methods. However, matching layers could increase the mass and size of the transducer and more importantly, distort the wave field received by the transducer. So this work is focusing on design electrical impedance matching network to maximum the power delivered to the substrate.

A linear phased array transducer (PAT) made of piezoelectric fiber composite (PFC) is chosen for which the electrical impedance matching network is built. The electrical impedance of each elements within the transducer is measured using impedance analyzer and it is identified there are two resonance peaks. The free vibration of the element has been modeled in finite element analysis and the vibrating modes of the two peaks are identified. For electrical impedance matching, a low pass T or PI network is chosen. For guided wave excitation, a broad bandwidth is desired. Thus, the impedance matching is performed at frequency range of 200 kHz to 800 kHz, given that the transducer is designed to have a

center frequency of 500 kHz. An initial guess of the value of components in the matching network is obtained by pick a value within the frequency range aforementioned and matched the impedance at that frequency to the 50Ω source load using the Smith Chart. The quality factor Q is kept less than 2 to achieve a broadband response. However, matched impedance at one frequency does not guarantee it works well for other frequencies. The mean value of power gain over this frequency range is maximized using different optimization methods. The optimized values are used to do the circuit simulation and obtain the increased power compared with no-matching excitation.

To test the performance of matching network, a multi-physics finite element model is created in COMSOL which combines the piezoelectric and electric circuit model. The simulation results show that the power delivered to the piezoelectric element is increased by using the matching network and the amplitude of excited guided wave is also increased.

To verify this in experiment, the electrical matching network is fabricated using printed circuit board. Each channel has its own matching network and thus can work independently. Generally, the results show that the matching network helps increase the wave amplitude. Since guided wave excitation is not only a function of power delivered to the transducer but also depends on the characteristic of particular mode. Usually, the guided wave mode will have different attenuation at different frequency. As a sequence, the experimentally measured power of guided waves does not necessarily agree with the power spectrum predicted in the theoretical and finite element analysis.

Similar idea has been applied to PVDF transducer as well. PVDF transducer has much lower weight and thickness than PFC transducer. Additionally, it is flexible and can be easily mounted on curved surfaces. However, its low piezoelectric coupling coefficient makes its received signal very weak. A matching network is designed for PVDF transducer using the same method. Good improvement in the amplitude of received signal is observed.

In conclusion, phased array transducer has many advantages over single element transducer in SHM. However, its low excitation power could limit its actual application. Electrical matching network is designed and significantly improve the power of transducer. The effect of matching network on guided wave excitation is also studied. Similar method has been applied to PVDF transducer to increase the amplitude of receiver.

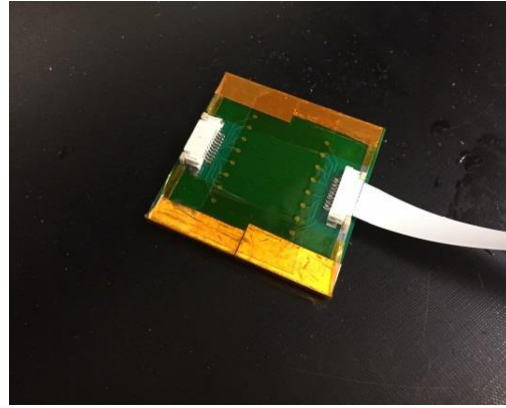
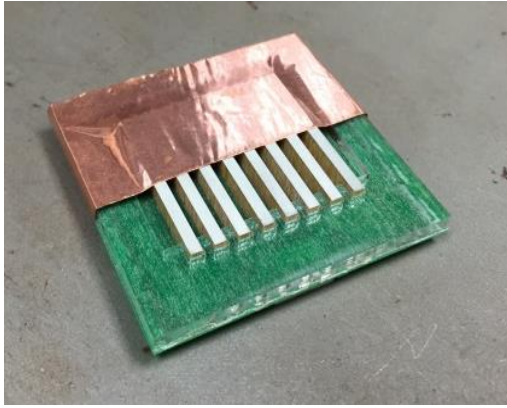


Figure 1: Phased array transducer for structural health monitoring

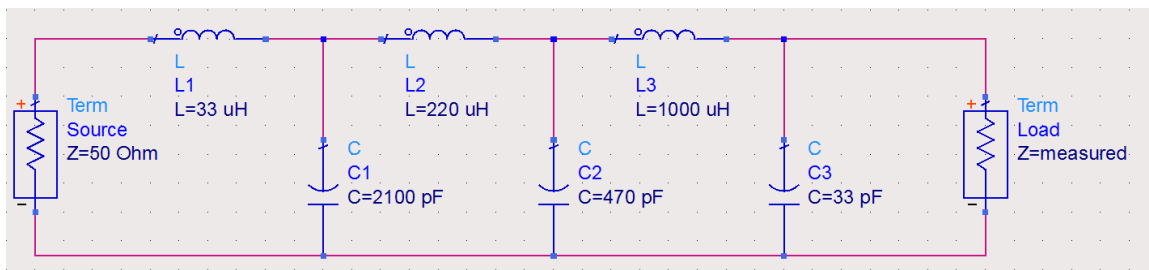


Figure 2: Designed matching network for the PAT transducer

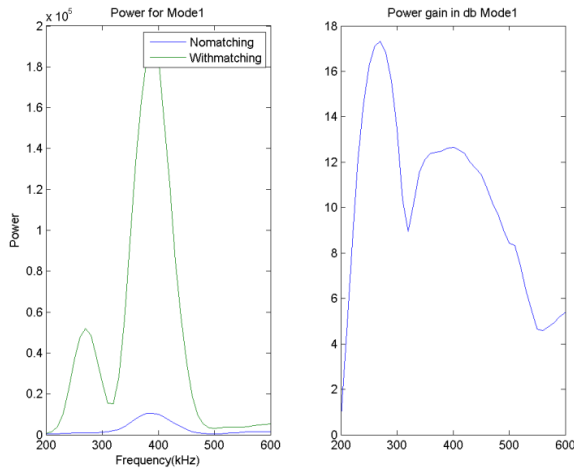


Figure 3: experiment results showing the power comparison in guided wave excitation with or without matching network.

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HYBRIDIZABLE DISCONTINUOUS GALERKIN METHODS FOR MODELING FLUID-STRUCTURE INTERACTION

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Modern scientific computing requires an ever increasing amount of detail and accuracy for simulating problems of practical importance, which in turn leads to increased costs in computational resources and time. This is even more true for the computational simulation of fluid-structure interactions (FSI), in which the tightly coupled multi-physics demands significantly more computational resources than traditional simulations. The burden is placed on the developer to optimize computational methods for maintaining high order accuracy while also minimizing computational cost. In this, the choice of model and discretization strategy can greatly affect the properties of the simulation.

There are several commonly used approaches available for numerically modeling partial differential equations, including finite difference methods, finite volume methods, and finite element methods. We choose to study the recently developed hybridizable discontinuous Galerkin (HDG) methods [1], specializations of discontinuous Galerkin (DG) finite element methods. DG methods have many positive qualities, including being locally conservative, scaling well at high-orders, and maintaining stability for a wide variety of problems [2]; however, their main downside is an increased number of degrees of freedom (DOFs) at cell interfaces and vertices, compared to continuous methods. These extra DOFs lead to increased computational costs, causing many to disregard DG methods for being too expensive. Hybridizable discontinuous Galerkin methods were developed in order to overcome this criticism.

By hybridizing the solution into local element solutions and a global trace solution on the element interfaces, HDG reduces the number of globally coupled DOFs, along with the computational cost of solving the global system, while preserving

the benefits of DG methods. As they are fairly new, HDG applications have thus far been limited in scope to non-multi-physics scenarios such as elastodynamics [3] and Navier-Stokes [4] problems; however, all of the components necessary for HDG FSI are present and the largest remaining hurdle is coupling them together.

In our previous work, we implemented and compared three different FSI coupling strategies (ways to combine the disparate solid and fluid models into a coupled FSI model) using standard CG finite elements [5, 6]. As monolithic coupling, which solves the governing equations for all physics models simultaneously, performed best in our CG simulations, we plan to move forward using it for HDG FSI. We present preliminary work towards the realization of a hybridizable discontinuous Galerkin finite element method for monolithically coupled fluid-structure interaction.

HDG formulations are presented for linear elastostatics for mesh motion, dynamic hyperelasticity for the solid, and arbitrary Lagrangian-Eulerian Navier-Stokes for the fluid. These are then combined into a monolithically coupled FSI formulation. We present verification of these individual components through the method of manufactured solutions, results for example problems solved with the individual components, and finally some preliminary HDG FSI results. We conclude by discussing our ongoing research plan for the future. Some of the areas we plan to explore are effects from variation of the stabilization parameter, difficulties in turbulence modeling for high Reynolds number flow, potential challenges for massively parallel simulations, and comparison with other FSI methods (e.g., partitioned coupling, continuous Galerkin, etc.). Determining conditions where the most computationally efficient method is HDG FSI is of particular interest.

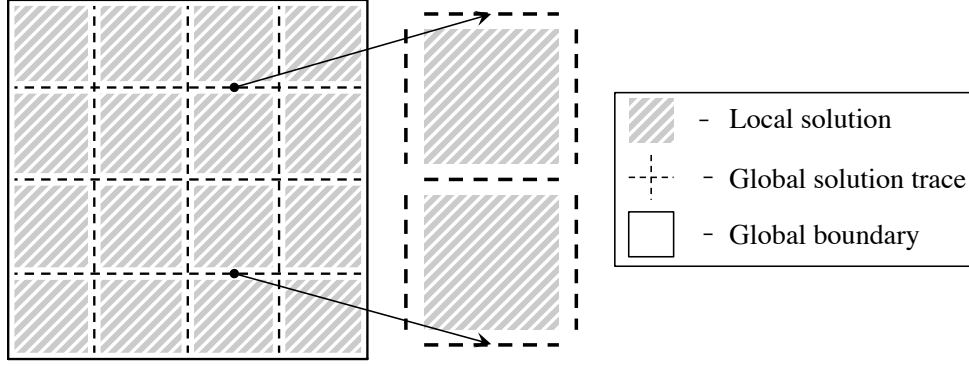


Figure 1: Domain illustrating the separation of the local solutions and the global solution trace. The local solutions are internal to each cell with no communication between cells, while the solution trace is global but exists only on the cell interfaces and the global boundary, where boundary conditions are applied.

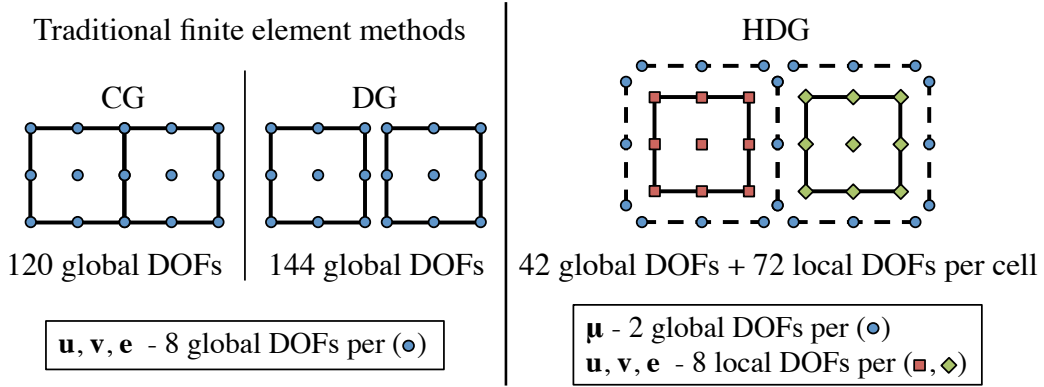


Figure 2: An example illustrating the global DOF reduction for HDG methods, using two 2D quadratic elements. In this example, $\mathbf{u}$ is displacement, $\mathbf{v}$ is velocity, $\mathbf{e}$ is strain, and $\boldsymbol{\mu}$ is global displacement trace. As seen, DG methods require more global DOFs than CG methods, and although at first appearances HDG methods require even more, very few of these are globally coupled (only $\boldsymbol{\mu}$), which results in a small system that needs to be solved globally. The local DOFs can be solved per cell in an inherently parallel fashion. These effects are even more pronounced for real problems with larger meshes, which are in 3D, and/or have higher order elements.

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THERMAL PROCESSING OF RECOMBINANT SQUID PROTEINS FOR MATERIALS FABRICATION

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Squid ring teeth ^[1] (SRT) is a semi-crystalline protein complex ^[2] extracted from the tentacles of the squid suction cups that exhibit a reversible transition (*i.e.*, thermoplastic) from a rigid to a rubbery material and, therefore, can be thermally shaped into any 3D geometry (*e.g.*, fibers, colloids, and thin films) ^[3]. Recently, Next Generation Sequencing in conjunction with high throughput proteomics were introduced ^[4] to rapidly identify genes that encode for SRT proteins. This sets the stage for heterologous expression, purification, and materials processing. Hence, recombinant bacterial expression of SRT proteins has been demonstrated ^[5]. These proteins have been shown to have excellent mechanical properties in both wet and dry conditions, exceeding most natural and synthetic polymers while having the unique capability of being thermally shaped into various functional forms. SRT proteins have segmented copolymer architecture with crystalline and amorphous domains, and a sequence-structure-property relationship that allows for tunable properties. Both its manufacture and its applications lend themselves well to environmental life cycle and overall sustainability. Being a biodegradable material (*e.g.*, enzymatic degradation), it not only reduces energy demands in

manufacture but also provides a renewable plastic for environmental protection. Deployable technology via fermentation reinforces its commercial and environmental sustainability (rather than relying on temporally-costly supply chain logistics).

Here, we studied the mechanical properties of recombinant SRT proteins via thermal and spectroscopic characterization techniques. A network model is proposed to explain the resulting thermo-mechanical response. Based on these results, we demonstrated extrusion, injection molding and hot-melt processing of a high strength recombinant SRT protein for the first time. SRT protein benefits include: (i) strong mechanical properties (*i.e.*, ~1GPa modulus) due to semi-crystalline molecular structure, (ii) reduced weight compared to carbon based fibers (density of 1.35 g/cm³ v.s. 1.8 g/cm³), (iii) reduced energy demands for fiber production (~20 kcal/g for plastics compared to ~10 kcal/g for recombinant expression), (iv) biodegradability, which addresses an increasingly significant goal of reduced environmental footprint and sustainability, (v) processing versatility (extrusion, injection molding, casting, etc.), and (vi) novel materials synthesis

strategy based on the “sequence (gene)-structure-property” relationship that will create tunable physical properties. Manipulating the protein network structure of SRT could help to develop novel material properties emerging from the atomic scale, and how to retain in much larger product-scale for materials fabrication. Thermoplastic SRT proteins hold great promise to provide a broad range of solutions due to their ability to soften in mild conditions and hence could eliminate the solution processes for industrial processes. Thermoplastic processes, used in the plastics industry, are preferred because drying steps could be eliminated; thus reducing their process time. Several attempts to commercialize recombinant silk-based fibers in the last two decades have failed because these could

only be produced using solution-based methods. This represents the biggest obstacle when trying to produce strong, pliable and durable fibers from recombinant silk. Utilization of extrusion and injection-molding technologies in SRT manufacturing offer the advantages of low cost and versatile processing. Both SRT and silk proteins are environmentally superior alternatives to synthetic plastics, will minimize waste and pollution, if the cost of production can be reduced. However, direct extraction of these proteins from natural resources is limited due to price. Therefore, recombinant expression is absolutely required for economically feasible and sustainable protein based production.

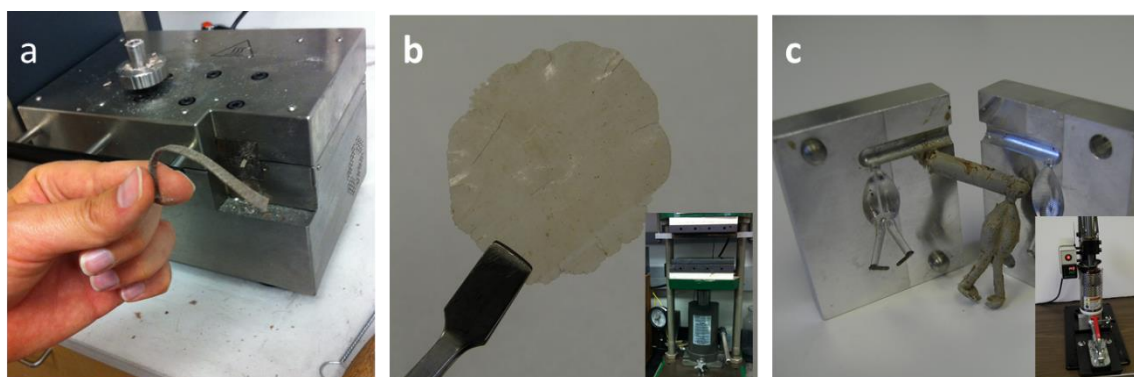


Figure 1: thermoplastic processing of recombinant SRT protein by extrusion (a), hot pressing (b) and injection molding (c).

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QUALITY OF LATENT SEBACEOUS FINGERPRINTS DEVELOPED WITH THIN FILMS OF DIFFERENT MORPHOLOGIES

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No crime can occur without the criminal leave a trace. As this is the underlying principle of modern criminalistics, forensic examiners try to uncover incriminating evidence left behind on various objects at crime scenes. Evidentiary fingerprints are particularly useful in either eliminating or identifying suspects because (i) no two persons have been known to have identical fingerprints and (ii) the ridge-and-valley pattern of a fingerprint does not change with age. Classification of the ridge-and-valley topology into a finite number of recognizable categories forms the basis of criminal identification systems today.

A latent fingerprint has to be developed for visualization and subsequent identification. Typically, physical or chemical techniques are used to develop a latent fingerprint left behind on a nonporous substrate. A common physical technique is to coat the sebaceous emulsion by an appropriately colored powder. Latent fingerprints are often chemically developed by chemical reactions deep within the residue. Fuming with cyanoacrylate is also a commonly used chemical development technique. A very thin film of zinc or cadmium deposited on a latent fingerprint impregnated with gold nuclei is sometimes used for by forensic examiners for development, especially when if the print is laid on a plastics substrate. Infrared-chemical imaging and mass spectroscopy are also emerging development techniques.

None of the aforementioned techniques visualizing latent fingerprints takes advantage of the ridge-and-valley topology of the fingerprint residue, but a new visualization technique does exactly that by conformally coating the top of a latent fingerprint by a columnar thin film (CTF) [1]. A CTF is an assembly of parallel nanocolumns typically grown by physical-vapor-deposition techniques such as thermal evaporation, electron-beam evaporation, sputtering, and ion-beam-assisted evaporation. For visualization of a latent fingerprint suspected to be lying on a substrate, a collimated vapor flux is generated by resistively heating a source material in a low-pressure

vacuum chamber and directed obliquely toward the substrate which is rotating rapidly about a central normal axis [2]. The source material is a metal, inorganic oxide, glass, or even an organic compound, depending on the substrate material. Upright nanocolumns macroscopically conform to the valleys and the ridges, the shadowing of very steep gradients during deposition being of little consequence for visualization. The coated fingerprint can then be seen by the naked eye and its optical image manipulated by specialized software.

Therefore, we decided to objectively compare three different types of thin films for development of latent fingerprints on nonporous substrates. The three types of thin films are morphologically categorized as Type 1 (upright nanocolumns), Type 2 (tilted nanocolumns), and Type 3 (dense thin film). The types of films can be seen in Fig. 1. Cross-section FE-SEM images of fingerprints developed by the deposition of all three types of thin films are shown in Fig. 2 [3].

Sixteen fingerprints halves were developed with each type of thin film, the multiplicity of samples helping to capture the natural variations of contact pressure when fingerprints are left behind as the fingerprint residue. Side-by-side comparisons of fingerprints developed by the three types of thin films are shown in Fig. 3. The percentage areas of clarity maps colored red (debatable ridge flow), yellow (debatable minutiae) and green (definitive minutiae) are presented in Fig. 4. The background was excluded for the calculation of the percentages. Fingerprints developed with type-1 thin films resulted in the greatest area of definitive minutiae with a mean of 36.67% and the least area of debatable ridge flow with a mean of 32.14%. The corresponding figures were 28.81% and 36.88% with type-2 thin films, and 17.44% and 50.41% with type-3 thin films. The mean area of debatable minutiae was about 30% for all three types. The data for both the red and green portions confirm that Type-1 film is the best performer and Type-3 film is the worst.

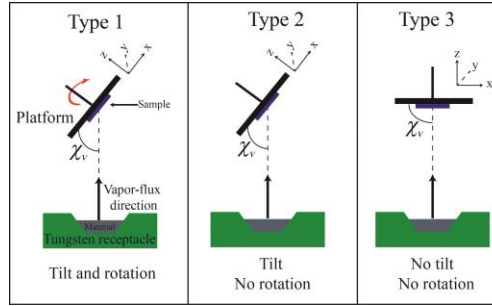


Figure 1: Schematics illustrating the deposition of thin films of three types on latent fingerprints laid on either glass slides or silicon wafers. Type 1: The platform was tilted so that $\chi_v = 20^\circ$ and rotated at 120 RPM. Type 2: The platform was tilted so that $\chi_v = 20^\circ$ but was not rotated. Type 3: The platform was oriented so that $\chi_v = 90^\circ$ but was not rotated

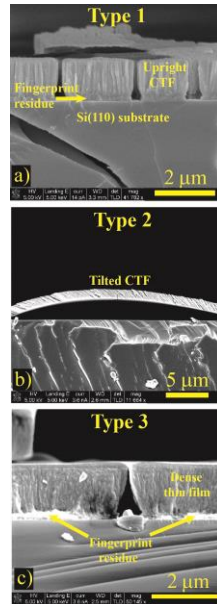


Figure 2: FE-SEM images of (a) a fingerprint coated with a type-1 thin film, (b) a type-2 thin film, and (c) a type-3 thin film.

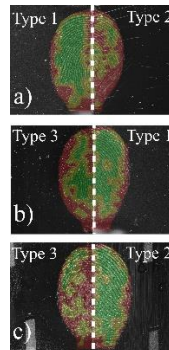


Figure 3: Clarity maps of left and right halves of three fingerprints developed by the deposition of thin films of three different types. (a) Types 1 and 2, (b) 3 and 1, and (c) 3 and 2. The areas of debatable ridge flow, debatable minutiae, and definitive minutiae are colored red, yellow, and green, respectively, while the background is colored black.



Figure 3: Percentage areas classified with debatable ridge flow (“DRF,” red circles), debatable minutiae (“Deb M,” dark yellow triangles), definitive minutiae (“Def M,” green squares) on 48 fingerprint halves developed with thin films of type 1, 2, or 3.

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Higher Harmonic Generation of Ultrasonic Waves due to Interaction with Microstructure

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Guided waves propagate along a boundary and can be used for inspection of longer distances than bulk waves, but as multiple modes can be excited, consideration must be placed into proper mode selection and excitation design. Higher harmonics are generated when a sinusoidal wave propagates through a nonlinear elastic media due to the interaction with the microstructure. These higher harmonics have been shown to be quite sensitive to microstructural features such as dislocation substructures, persistent slip bands, precipitates, etc. Hence, there is potential in the use of higher harmonics of ultrasonic guided waves analysis as a tool to nondestructively inspect/detect damages such as fatigue in metallic structures, creep-fatigue damage in components in nuclear plant, and stress corrosion cracking in used nuclear fuel dry storage canister at an earlier damage state compared with conventional ultrasonic guided wave techniques. Evidently, progressive damage is expected to occur from microscale and eventually project to macroscale changes, hence changes the degree of nonlinearity can be due to material damage contributions. Differentiating material contributions from system contributions must be resolved.

We will highlight our recent progress on theory, numerical simulations, and laboratory experiments to develop higher harmonic guided waves as a tool to detect microstructural changes that precede macroscale damage. Analyzed structures include plates and hollow cylinders, and we focus on localized damage initiation. These recent experiments focus on using magnetostrictive transducers in activating the fundamental shear horizontal mode (SH0) and the third harmonic that is generated due to the material nonlinearity. The magnetostrictive transducer comprises a thin iron-cobalt foil, a meandering electric coil, and a permanent magnet. These transducers are inexpensive, easy to use, and are very efficient at generating shear waves. In applications where the wavelength is larger than the plate thickness, the waves are guided by the traction free boundary conditions and propagate in the plane of the plate. The SH0 mode is nondispersive and generates a third harmonic of the same mode that is shown to be sensitive to localized plastic strain and unseen fatigue damage. In addition, the cumulative nature of specific primary-higher harmonic mode pairs was verified and deviation from normalized modal amplitude ratio trend demonstrated the influence of localized plastic deformation.

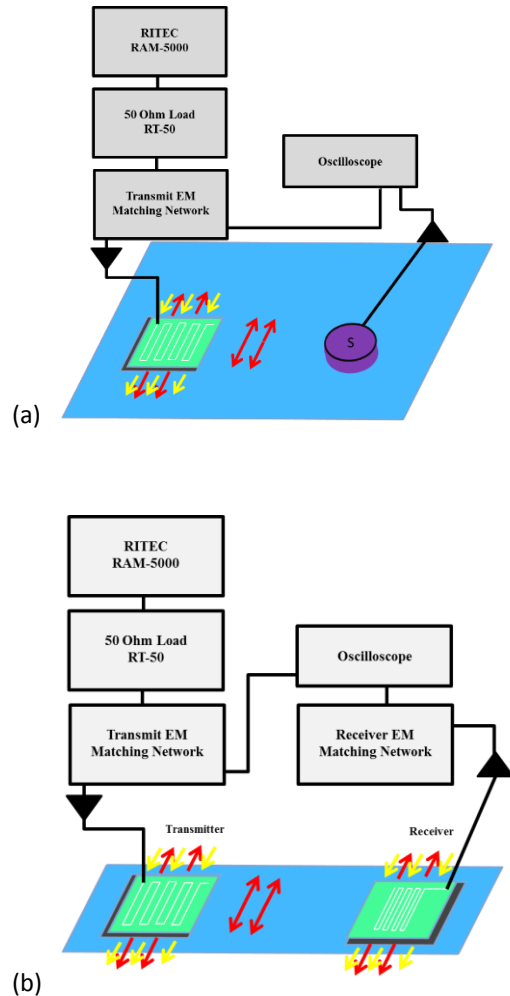


Fig. 1. Schematic of experimental test setup for investigating SH0/sh0 primary/third harmonic (a) cumulative trend and (b) trend in deformed plates. Meander coils for transmitter and receiver configuration respectively have wavelengths of 3.6 and 1.2 mm

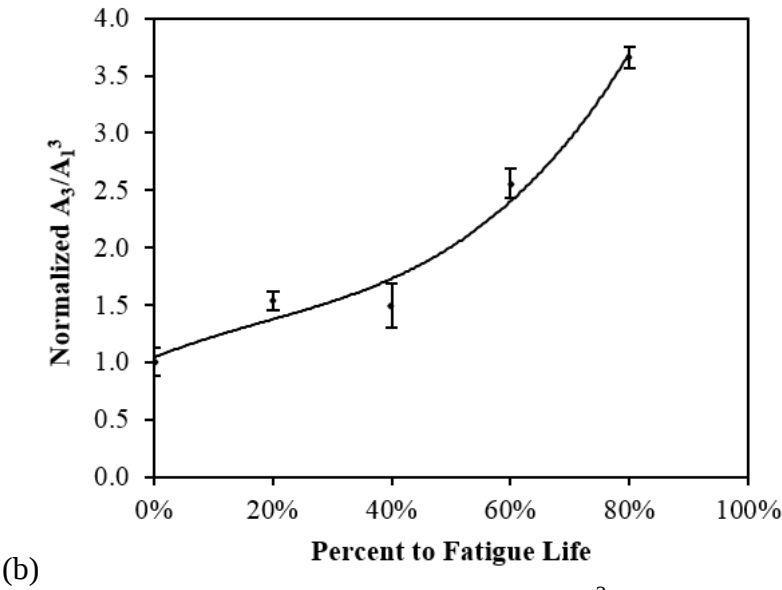
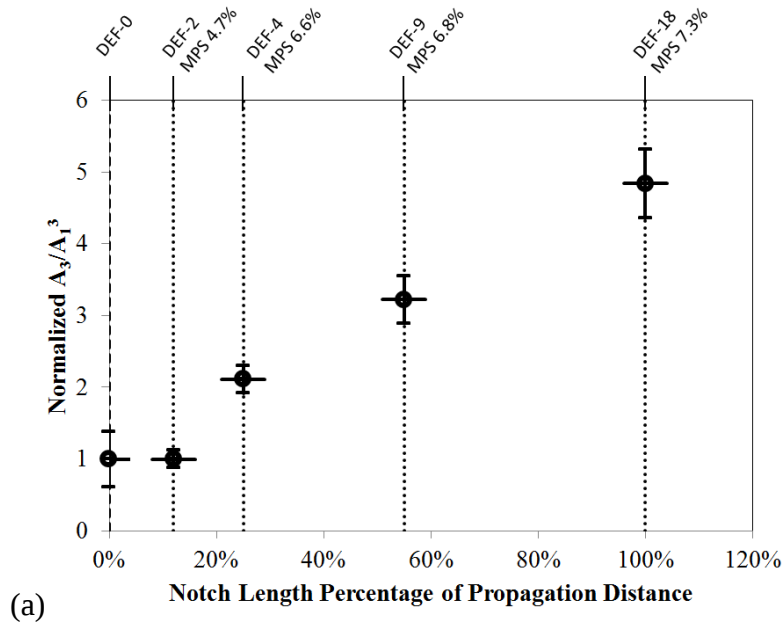


Fig. 2. (a) Normalized modal amplitude A_3/A_1^3 for specimens that were quasi-static tensile plastic deformation with different gage lengths. [1]. (b) Normalized modal amplitude for five different fatigue specimens. [2]

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Verification of Reduced-Order Modelling Codes with Truncated Bases

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In recent years, simulations have become an increasingly important part of the engineering design process. This has caused a demand for the ability to compute solutions that are both accurate and computationally affordable. High-accuracy simulations consist of linear systems with degrees-of-freedom numbering in the millions. For example, a high-fidelity simulation of the flow in a turbine engine can be very computationally expensive and take on the order of weeks to compute. Running high-fidelity simulations can form a bottleneck in the design process. Reduced-order models derived from high-fidelity simulations offer a way to alleviate the bottleneck.

One reduced order modeling technique is to use snap-shots from a high-fidelity simulation to derive a reduced order basis. The reduced order basis is significantly smaller than the basis used in the high-fidelity simulation. The governing equation is then projected onto the reduced order subspace. By working in a much lower dimensional subspace, significant computational savings are reaped.

There are several techniques for deriving a truncated set of basis vectors. A common one that will be used here is the technique of Proper Orthogonal Decomposition (POD) [1], but it is far from being the only one.

There are also various techniques to use a truncated basis to solve problems. Once a reduced order basis has been chosen, it can be used as the basis vectors in the finite element method to solve differential equations. For example, basis vectors can be derived using Proper Orthogonal Decom-

position and then used with the Galerkin finite element method to solve a differential equation [1, 2]. This particular method is often referred to as the POD/Galerkin method in literature.

With either a full-order or a reduced-order model, it is important to verify that the equations and numerics were correctly implemented into a computer code. There are well developed techniques for rigorously verifying full-order models such as the method of manufactured solutions [3]. However, this technique cannot be applied to a reduced-order models with an incomplete basis because the error might not converge to zero.

To address the problem, we present a method for verifying reduced-order models of truncated bases. To the best of the author's knowledge, there is not a verification strategy to confirm the implementation of numerical methods that utilize a truncated set of basis vectors such as the POD/Galerkin method. The goal of the research was to develop a technique for verifying the POD/Galerkin method. This way, developers can have confidence the code they are using is giving correct mathematical results.

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SURFACE ACOUSTIC WAVE DRIVEN ACOUSTOPHORESIS

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Surface Acoustic Wave (SAW) based systems have gained prominence in recent years for various lab-on-a-chip applications including particle and fluid manipulation. However, the theoretical and numerical work on SAW is rather limited and so is the full understanding of the fundamental physical mechanisms, e.g. what is the mechanism behind the vertical focusing of particles in polydimethylsiloxane (PDMS) channels driven by SAW [1] and what is the critical particle size for the transition between radiation-dominated and streaming-dominated acoustophoresis in these systems? The latter has been extensively studied for Bulk Acoustic Wave (BAW) driven systems numerically by Muller *et al.* [2] and experimentally by Barnkob *et al.* [3] In this work, we present a numerical analysis along the lines of that by Muller *et al.* [2], but where the model differs in the actuation mechanism and the wall conditions. Figure 1 shows a schematic of a typical device for SAW separation in a PDMS microchannel. We model the fluid using compressible Navier-Stokes equations without making any *a priori* assumptions about specific flow regimes. We employ a perturbation approach where the solution of the first-order equations is used to calculate the source terms in the time-averaged second-order equations, which are then solved to obtain the acoustic streaming field. Combining information from these two solutions, it is possible to estimate the mean trajectory of particles in the flow. The particle motion inside the flow is governed by two forces: acoustic radiation force, F_{rad} , and the hydrodynamic drag force from the acoustic streaming. In most acoustofluidics problems the inertia of the bead can be neglected and thus, the velocity of the particles can be obtained using Newton's second law. We apply impedance boundary conditions to model the PDMS channel walls, while the bottom surface of the channel is subjected to a standing SAW. This actuation displacement is obtained via superposition of two SAWs traveling in opposite directions using the traveling SAW displacement profile. The numerical solution was obtained via an in-house finite element code based on the *deal.II* finite element library. Figure 2 shows the plots of the first-order and second-order fields. These fields are significantly different from those obtained by Muller *et al.* [2] for BAW systems, which can be attributed to the large differences in acoustic

impedance of the channel wall material (PDMS for SAW systems versus typically glass or silicon for BAW systems). Specifically, the first-order fields in SAW systems are characterized by traveling waves across the channel height as opposed to the standing waves observed in BAW-driven systems. Figure 3 shows the trajectories of polystyrene particles of diameter (b) 1 μm , (c) 5 μm , (d) 10 μm , (e) 15 μm , and (f) 20 μm . It can be seen that while the motion of the smaller particles is dominated by the hydrodynamic drag force, the motion of the large particles is radiation force driven and large particles are moved to the pressure node by the acoustic radiation force. The critical size for transition from streaming dominated motion to radiation force dominated motion obtained from our numerical model is similar to those reported by experiments which have shown the ability of SAW devices to separate particles of size around 7 μm due to the radiation force. We also observe vertical focusing of larger beads, which in combination with gravity (neglected in this work), may explain the results obtained by Shi *et al.* [1] Future investigations will aim at more comprehensive validation of our numerical model using 3D astigmatic particle tracking measurements to gain a better understanding of the acoustophoretic phenomena in SAW devices. Such experimental verification would pave the road for further enhancements of our numerical model to include wall enhancement effects of the viscous drag force as well as the inclusion of the heat-transfer equation in the governing equations in order to account for temperature effects.

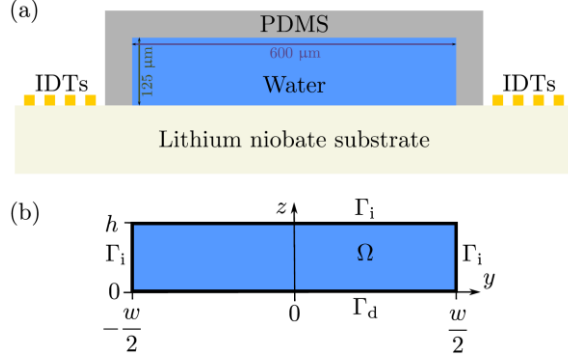


Figure 1: (a) Cross-sectional sketch of the SAW-driven device consisting of a lithium niobate substrate and liquid-filled PDMS channel (width $w = 600_\mu\text{m}$ and height $h = 125_\mu\text{m}$). The substrate is acoustically actuated via two sets of interdigitated electrodes (IDTs). (b) Sketch of the computational domain Ω with impedance boundaries and Dirichlet actuation boundary.

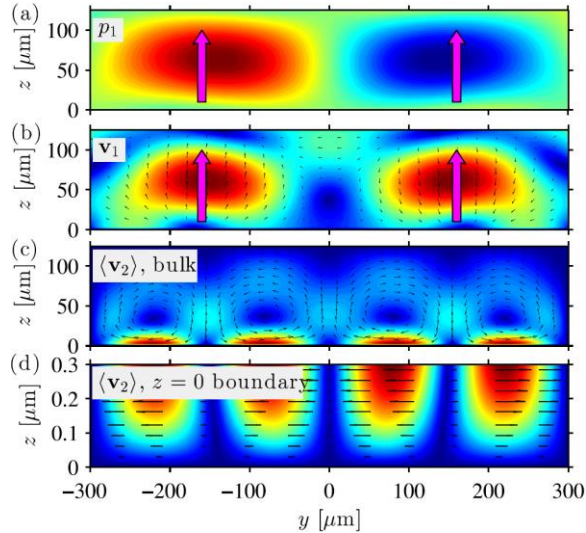


Figure 2: (a) Oscillating first-order pressure field, p_1 [colors ranging from -12.9 kPa (blue) to 12.9 kPa (red)]. (b) Oscillating first-order velocity field $\mathbf{v}_1$ [magnitude shown as colors ranging from zero (blue) to 8.11 mm/s (red), vectors shown as black arrows]. (c) Time-averaged second-order velocity field, $\langle \mathbf{v}_2 \rangle$, bulk [magnitude shown as colors ranging from zero (blue) to 1.83 mm/s (red), vectors shown as black arrows]. (d) Zoom of the time-averaged second-order velocity field $\langle \mathbf{v}_2 \rangle$, $z = 0$ boundary.

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field $\langle \mathbf{v}_2 \rangle$ in (c) in a slab of $0.3 \mu\text{m}$ height from the bottom wall.

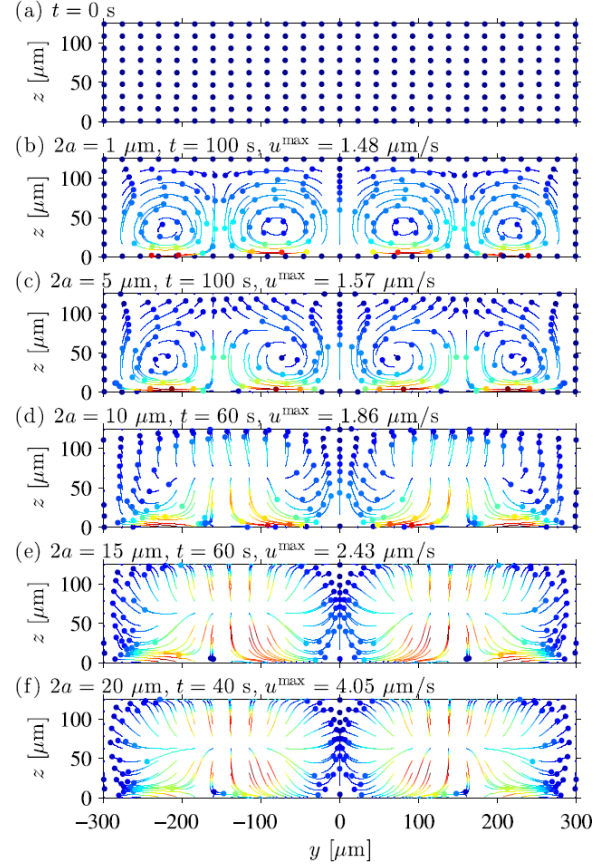


Figure 3: Particle trajectories with particle velocities as colors from blue minimum to red maximum and colored disks denoting the final positions within the observation time. (a) Starting position of 175 particles distributed uniformly within the microchannel. The panels (b)-(f) show the trajectories of (b) $1 \mu\text{m}$ particles during 100 s, (c) $5 \mu\text{m}$ particles during 100 s, (d) $10 \mu\text{m}$ particles during 60 s, (e) $15 \mu\text{m}$ particles during 60 s, and (f) $20 \mu\text{m}$ particles during 40 s. The motion of the smaller particles is dominated by the viscous drag force from the acoustic streaming, while the larger particles are pushed to the pressure nodes by the acoustic force.

Multilayer Transfer Matrix Characterization of Complex Materials with Scanning Acoustic Microscopy

Jeong Nyeon Kim, Dr. Richard L. Tutwiler, and Dr. Judith A. Todd

Abstract

Multi-layered structured thin film systems, such as those used in biomedical thin films, MEMS (Micro Electric Mechanical Systems) / NEMS (Nano Electric Mechanical Systems) devices, and semi-conductors are widely used in various industries. In recent years, the mechanical scanning acoustic reflection microscope has become well instituted as a useful non-destructive tool for evaluating multilayered structured thin film systems. In particular, the $V(z)$ curve method with the scanning acoustic microscope can be used to characterize a very small area of the system. In this study, $V(z)$ curve simulation software for simulating the transducer output when an ultrasound wave is transmitted into the specimen has been developed. The Thompson-Haskell transfer matrix method was applied to solve for the reflectance function in the software. All input and output interfaces were incorporated in a GUI for convenience of the users. Surface acoustic

wave velocities were calculated from the simulated $V(z)$ curves. For precise calculation, signal processing techniques were utilized. The surface acoustic wave velocities were compared to those from an experiment with a bulk solid. The simulation's thickness sensitivity was also tested with different thicknesses at the nanoscale. A series of experiments with multilayered solids were carried out and the results were compared with the simulations. Furthermore, nano-scratch tests were conducted on the multi-layered materials and their critical loads were compared with the $V(z)$ curve measurement results. These results represent the first comparison of analytical versus experimental data for $V(z)$ curves for multilayered systems. For the multi-layered specimens, silicon (100) was used as a substrate. Titanium (thickness: 10 nm) and platinum (thickness: 100 nm) were deposited, respectively.

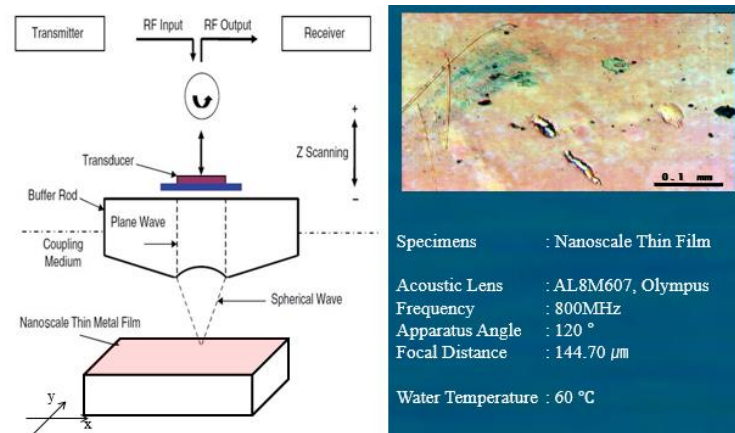


Figure 1. Schematic of scanning acoustic microscope and an example of ultrasonic image

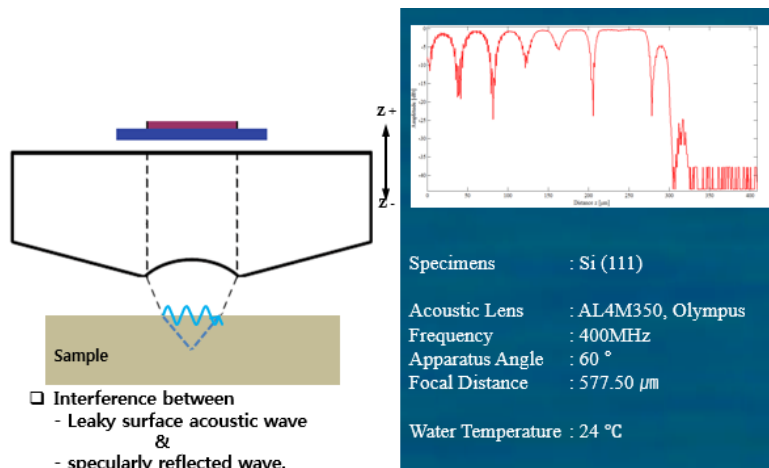


Figure 2. Schematic diagram of $V(z)$ curve measurement and an example of $V(z)$ curve.

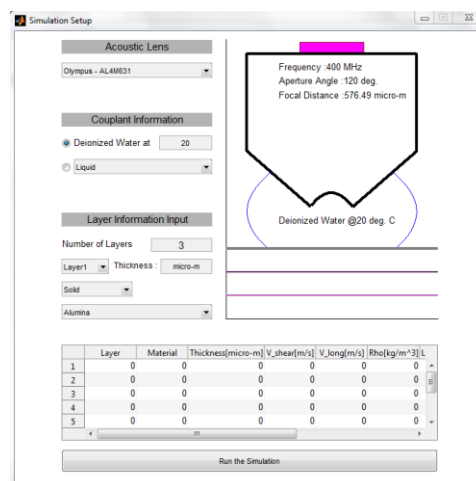


Figure 3. A screenshot of $V(z)$ curve simulation program – Simulation setup window.

The circular Bragg phenomenon for oblique incidence

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Abstract

Structurally chiral materials exhibit the circular Bragg phenomenon (CBP). These materials preferentially reflect circularly polarized light of the same handedness while transmitting circularly polarized light of the opposite handedness within a range of wavelengths called the circular Bragg regime. The CBP has been extensively investigated experimentally for normal incidence, but not for oblique incidence. After fabricating a 20-period-thick chiral sculptured thin film, we measured all of its circular remittances over a 60° range of the angle of incidence and a 300-nm range of the free-space wavelength. Provided the incidence is not very oblique, the obtained dependencies of the center wavelength and the bandwidth of the CBP on the angle of incidence match theoretical estimates.

Introduction

The circular Bragg phenomenon (CBP) is exhibited by structurally chiral materials such as cholesteric liquid crystals (LCs) and chiral sculptured thin films (STFs) [1, 2]. Circularly polarized light of the same handedness is preferentially reflected over circularly polarized light of the opposite handedness within a range of free-space wavelengths called the circular Bragg regime, by these materials. The circular-polarization-selective reflection is extensively exploited in optics [3]. Experimental research on the CBP has been largely confined to normally incident light, and measurements directly

related to the exhibition of CBP for oblique incidence are rarely reported in the literature, as becomes clear from a recent review [3]. This lacuna prompted us to experimentally investigate the variations of the center wavelength λ_0^{Br} and the full-width-at-half-maximum FWHM bandwidth $\Delta\lambda_0^{\text{Br}}$ of the CBP of a chiral STF with respect to the angle of incidence θ .

Materials and Methods

A chiral STF was deposited on a pre-cleaned microscope glass slide by thermal evaporation in a low-pressure chamber using the serial bidepositon (SBD) technique [4]. ZnSe powder was placed in a tungsten boat, 15 cm above which was located the glass slide affixed to a rotatable holder. The chamber was pumped down to a base pressure of 0.2 μTorr . After 95-A current began to be passed through the boat to heat the ZnSe powder resistively, the substrate was oriented such that ZnSe vapor flux arrived at an angle of 25° with respect to the exposed surface of the glass slide. During deposition, the SBD technique was implemented to grow the chiral STF. Both the circular reflectances (R_{RR} , R_{LL} , R_{RL} , and R_{LR}) and the circular transmittances (T_{RR} , T_{LL} , T_{RL} , and T_{LR}) of the chiral STF were measured as functions of the free-space wavelength $\lambda_0 \in [600, 900]$ nm using a custom-made variable-angle spectroscopic system. The first subscript is the circular polarization state of the reflected or transmitted light and the second subscript is the circular polarization state of the

incident light. The circular reflectances were measured for $\theta \in [10^\circ, 70^\circ]$, and the circular transmittances for $\theta \in [0^\circ, 60^\circ]$.

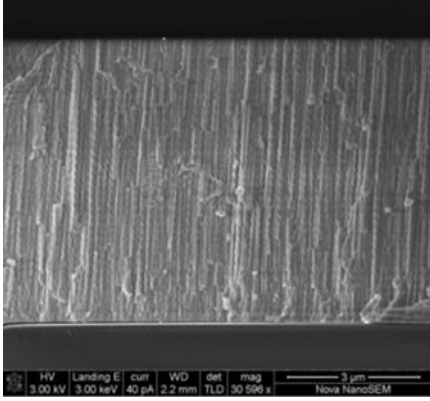


Figure 1. Scanning electron micrograph of the fabricated chiral STF.

Results and Discussion

The fabricated chiral STF was structurally right-handed and possessed 20 periods in the thickness direction, each period being 325 nm, according to the cross-sectional scanning-electron micrograph in Fig. 1. From the measured spectrums of the circular remittances of this chiral STF, we determined that the dependencies

$$\lambda_0^{\text{Br}}(\theta) \propto 3.2157\cos^{1/2}\theta - 3.9444\cos\theta + 1.7205\cos^{3/2}\theta$$

$$\Delta\lambda_0^{\text{Br}}(\theta) \propto 2.1077\cos^{1/2}\theta - 1.1494\cos\theta + 0.0527\cos^{3/2}\theta$$

hold for $\theta \in [0^\circ, 60^\circ]$. Previously, analyses of theoretical results have suggested the simple estimates $\lambda_0^{\text{Br}}(\theta) \propto \cos\theta^{1/2}$ and $\Delta\lambda_0^{\text{Br}}(\theta) \propto \cos\theta^{1/2}$ for $\theta \leq 30^\circ$, when (i) dissipation is either mild or so weak as to be ignored and (ii) the number of periods is sufficiently large [2, 5]. Comparison with the experimentally determined equations indicates that both of these simple estimates indeed hold for $\theta \leq 30^\circ$, with errors not exceeding 10%. Thus, the obtained dependencies of the center wavelength and the bandwidth of the CBP on the angle of incidence match previously obtained theoretical estimates, provided that the incidence is not very oblique. This finding is of importance for angle tuning of circular-polarization filters made of chiral STFs [2, 3].

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EFFECT OF LOAD AND TEMPERATURE CHANGES IN STRUCTURAL HEALTH MONITORING USING NONLINEAR ULTRASOUND

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Use of nonlinear ultrasound for evaluating and monitoring micro-scale damage progression in materials has been studied for decades. Most of the earlier research focused on the contribution of dislocations to the second and third harmonic wave generation in bulk waves [1]. It later motivated many research to use nonlinear ultrasound for characterizing various types of damages namely, fatigue, thermal aging, creep damage, and radiation damage [2]. Recent advances in ultrasonic guided waves further make it possible to combine the penetration power of guided waves with the early damage detection capabilities of nonlinear ultrasound to interrogate a fairly large area [3]. Therefore, structural health monitoring (SHM) incorporating nonlinear ultrasound seems promising. However, there is a need to re-examine the definition of nonlinearity parameter associated with *in situ* SHM application. Since the β parameter is widely used to

quantify ultrasound wave distortion caused by microstructural damages, there exist some cases where the β parameter can change without significant microstructural damage accumulation. Most common examples include diffraction and attenuation. Therefore, other effects can come into play when incorporating nonlinear ultrasound into SHM. While the effect of diffraction and attenuation is studied [4], not many research have investigated the effect of load and temperature changes on nonlinear ultrasound. In this paper, we experimentally examined the effect of load and temperature changes on nonlinear ultrasound guided waves. The β parameter was examined from the shear horizontal (SH) mode wave in an aluminum 2024 plate undergoing increasing static in-plane stress at a constant temperature and increasing temperature under no load. The results and implication on SHM will be discussed.

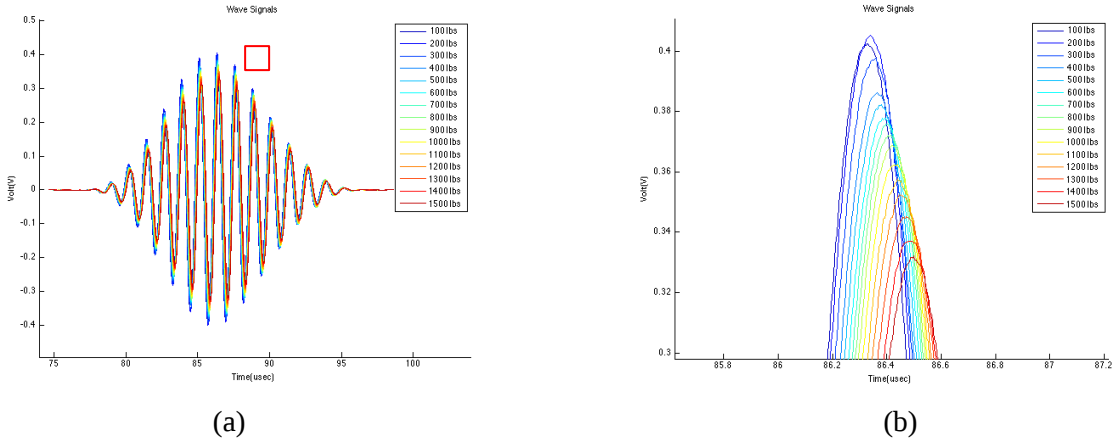


Figure 1: One complete set of wave signals obtained from the first run of increasing-load experiment is shown in the left (a), while the figure on the right (b) is a magnified view of the peaks denoted by the red rectangle on the left figure. From the figure (b), it is evident that the amplitude and the velocity of waves depend on the external in-plane load.

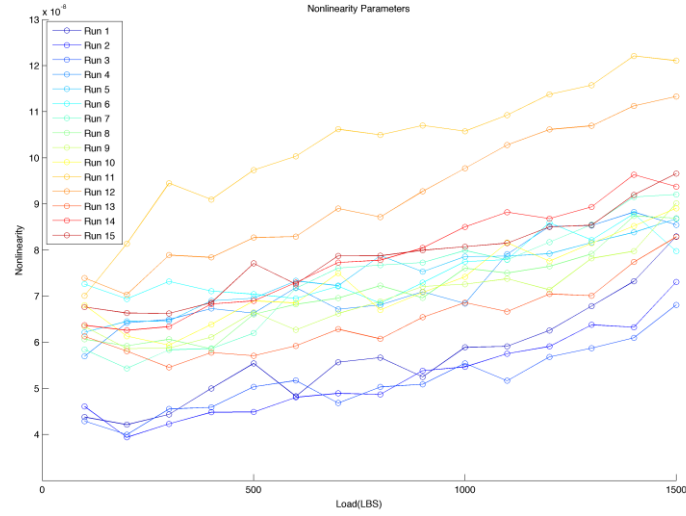


Figure 2: The measured nonlinearity parameters from the entire runs of increasing-load experiments are plotted in a figure. The nonlinear parameter is also dependent on in-plane load. This is mainly not because of increase of the third harmonic amplitude but significant decrease of the fundamental frequency amplitude.

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Cognition affects brain-computer interface utility in people with amyotrophic lateral sclerosis

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Brain-computer interface (BCI) assistive communication devices have the potential to enhance the quality of life for those with conditions causing central and peripheral nervous system dysfunction, including patients with amyotrophic lateral sclerosis (ALS). This disease is defined by motor neuron loss, resulting in impairments of movement, speech, swallowing, and respiration. Anatomical and genetic evidence supports ALS as part of a neurodegenerative syndrome associated with frontotemporal dementia; as a result, cognitive dysfunction and behavioral changes may manifest in up to half of ALS patients [1]. This study was performed to assess the effect of disease factors, including psychological impairments, on two BCI paradigms, the P300 speller and the motor-imagery task.

Twenty-five patients attending the ALS Clinic of the Penn State Hershey Medical Center were enrolled in this study, along with fifteen neurologically healthy control participants. Clinical data, including ALS Functional Rating Scale - Revised (ALSFRS-R), age, gender, time since symptom onset, and education level of the patients were recorded. The ALSFRS-R is a twelve item measure of physical function. Patients and controls were also administered the ALS - Cognitive Behavioral Screen (ALS-CBS), a brief neuropsychological screen to assess cognition and behavior [2].

Patient and control participants completed four and two sessions, respectively, of electroencephalogram (EEG)- based BCI recordings over the course of 1-2 months, with each hour-long session split between two BCI paradigms: a P300 spelling system, and a 2-class motor-imagery center-out task. In addition to the accuracy achieved during the online operation of the BCI tasks, the main measure of performance was the 'quality' of the control signal developed by each user. Quality

represents a classifier-independent measure of mental state discriminability, calculated as the standard distance between the data belonging to the two classes in each task. For the P300 speller this is the standard distance between the evoked potentials generated by target and non-target letters, and for the motor imagery task, the standard distance between band powers of 5-30 Hz for left and right imagery trials. To determine whether task quality was associated with physical or psychological factors, we performed two multiple linear regressions, with the quality scores as the dependent variables. The independent factors in these regressions were the motor, bulbar, and respiration sub-scores of the ALSFRS-R, as well as the behavioral and cognitive scores of the ALS-CBS.

Fourteen patients were defined as cognitively impaired, and eight as behaviorally impaired. The cognitive scores of the control group were significantly higher than the patients ($p = .013$). Accuracies were similar for patients and controls on the motor-imagery task., although controls achieved higher overall accuracy than patients on the P300 task ($p = .033$, Figure 1) On both of the BCI tasks, cognition was the only variable to significantly correlate with signal quality (Figure 2), implicating cognitive health, rather than physical factors, critical in BCI success. ANOVA and subsequent post hoc tests determined that patients with cognitive impairment possessed an elevated ratio of non task-relevant power to task-relevant power compared to the other two groups (Figure 3). This finding provides a possible mechanism for losses in performance observed in patients with cognitive impairment, although strategies for overcoming or circumventing this limitation are topics for future study.

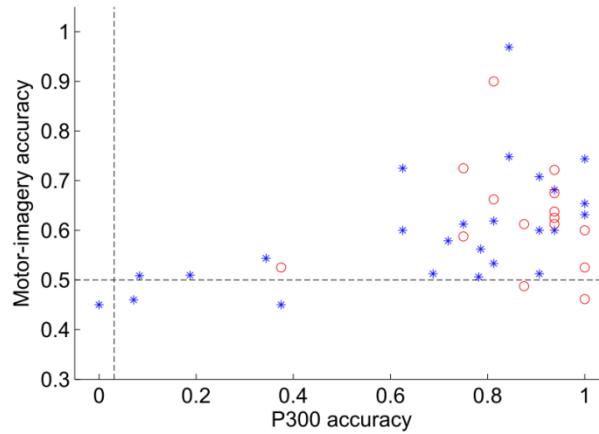


Figure 1: Online accuracy for patients (*) and control participants (o) for the P300 and motor-imagery BCI systems. Dashed lines denote the expected accuracy of random performance on each task.

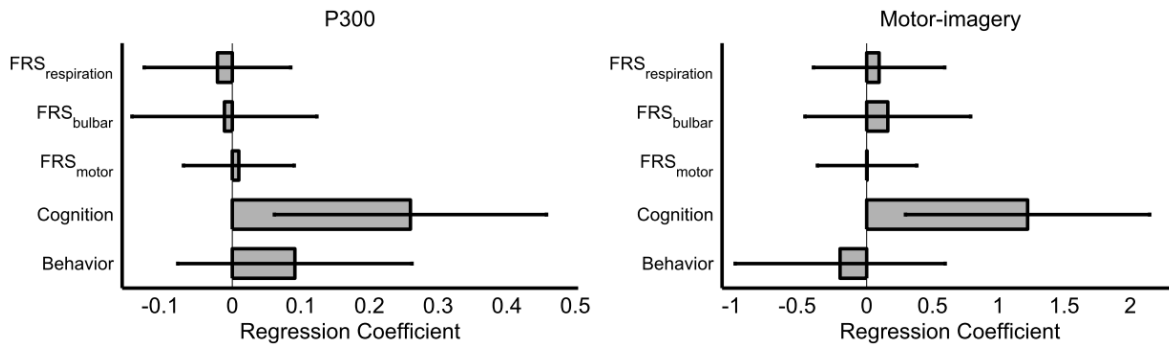


Figure 2: Cognition positively correlates with BCI signal quality. (Left) Regression of P300 quality on patient characteristics. Bars indicate the mean regression coefficients for each factor, along with 95% confidence interval of this estimate. (Right) Regression with motor-imagery quality as the dependent variable.

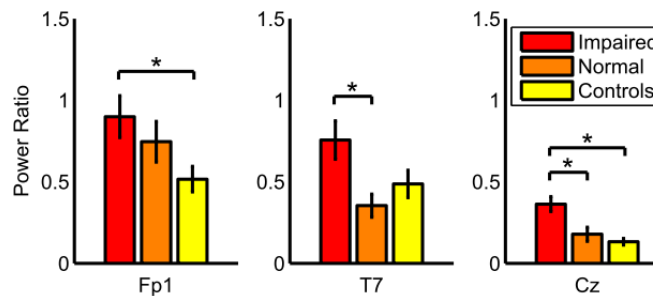


Figure 3: Cognitively-impaired patients display elevated ratios of power during rest trials in the 40 – 50 Hz band over the average power in the 8 – 24 Hz band in channels Fp1, T7, and Cz. Significant pairwise differences between groups at the $p<0.05$ level are indicated by an asterisk.

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STRESS EFFECT ON THE INITIAL LITHIATION OF SILICON NANOWIRES

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ABSTRACT

Silicon has been recognized as a promising anode material for the next generation of high-capacity lithium-ion batteries because of its high theoretical capacity. It is well-known that the electrochemical reaction in the crystalline Si nanowires (c-SiNWs) anodes is controlled by the migration of the interface accompanied with the solid-state amorphization through a ledge mechanism by peeling off of close-packed {111} atomic planes [1]. In this paper, we perform a reactive molecular dynamics simulation using the ReaxFF potential to study the lithiation process of a SiNWs. Reactive MD-simulation at high-temperature (900K) reveals that when lithium penetrates into the Si-NW in the $\langle 111 \rangle$ growth direction, a Li_xSi alloy shell is developed. The interlayer ([111] layers) Si-Si bonds break only at high Li atom concentration in the vicinity of these bonds, the amorphous-crystalline interface (ACI) is atomically sharp, and the lithiation proceeds by layer-by-layer peeling, in good agreement with experimental observations. Using stress analysis and ring statistics, we also show that slowing down of the reaction front (i.e. the phase boundary between the c-Si core and a- Li_xSi shell) propagation happens due to the retardation effect of the lithiation-induced compressive stress in the ACI layer. This result is in complete agreement with TEM images which exhibit the self-limiting of lithiation and formation of core-shell structure. The hydro-static stress at which the lithiation process no longer proceeds is measured from our simulations. Our modeling results shed light on the electrochemical insertion process of Li into high-capacity electrodes and provide fundamental guidance to the rational designs of the next generation high capacity electrode materials with enhanced capacity retention and durability.

2. RESULTS AND DISCUSSION

To elucidate the lithiation process in silicon nanowires, similar to the experimental settings [1], a crystalline Si $\{112\}\{111\}$ nanowire with 8.43 nm width and 9.22 nm heights, containing 5976 Si atoms, is considered as a representative volume element. As indicated in Figure 3, the $[1\bar{1}2]$ surface of nanowire is exposed to a lithium reservoir which is a block of randomly dispersed Li atoms, to mimic a-Li, on the top of the c-Si. Periodic

boundary conditions are applied along the planar x and y direction which correspond to the $[110]$ and $[111]$, respectively. Starting with NVT-MD simulations (constant volume and constant temperature using a Berendsen thermostat with a temperature-damping constant of 50 fs) the structure is initially minimized at very low temperature ($\sim 1\text{K}$) for 10ps to eliminate simulation artifacts which can arise from high energy contacts initially present in the starting geometry. Then the temperature was gradually increased until 900K with 18K/(1000 MD-iteration) rate (18K every 1000 iteration of MD) under NVT ensemble. Then, the obtained minimized system is subsequently equilibrated at 900K until the end of simulation. Figure 1 shows that during the amorphization process, the negative heat of formation of Li_xSi -phases causes the Li atoms invade the pristine Si $\{112\}$ surface, along $\langle 110 \rangle$ direction, and accumulate locally near the Li/Si phase interface by forming the first lithiated layer called reaction front. Note that since the solid-state diffusion of Li within the bulk c-Si network is associated with a substantial amount energy barrier, to overcome such barrier for long-range diffusion, our simulations have to be performed at elevated temperatures to allow observation of Li-diffusion events on the nanosecond time-scale accessible to ReaxFF-based MD simulations. Figure 1 also displays the morphological evolution of SiNW upon lithium intercalation. These results can be directly compared to the high-resolution TEM images reported by [1] (Refer to Figure 2). This figure clearly demonstrates that lithium invasion into c-Si NW takes place along the lateral $[110]$ and $[112]$ directions. The atomically resolved dynamical morphologies shown in Figure 4 evidently indicate their similarity to the geometries observed during high resolution TEM [1]. Additional lithium insertion occurs when Li-atoms occupy the remaining tetrahedral (Td) sites between two adjacent $(\bar{1}\bar{1}1)$ – planes consecutively and results in the breaking the Silicon atoms lying on the zigzag-like $(\bar{1}\bar{1}1)$ sites away.

We observe that each mono-layer of the $\{111\}$ surfaces is lifted-off when all four possible Td sites below the surface are filled and the interlayer Si-Si covalent bonds break. Dissolution of the dissociated c-Si layers through the lithium forms an amorphous layer of Li_xSi separated by a thin layer of lithiated silicon so called amorphous crystalline interface (ACI). Furthermore, it is understood from ab initio simulation of mixing Li and Si upon

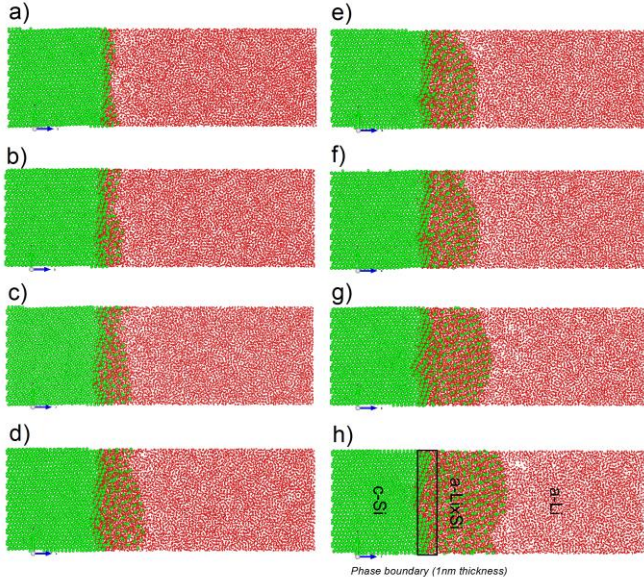


Figure 1: Atomistic mechanism of electrochemically-driven solid state amorphization. Snapshots from MD simulations showing the movement of an amorphous/crystal interface, which mimics the peeling-off process seen in experiments. Layer-by-layer peeling-off (Fig a-h) derives the solid state amorphization by ledge mechanism formation.

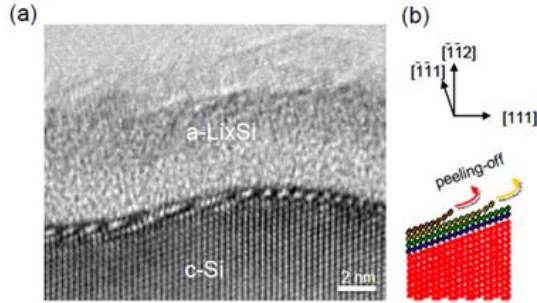


Figure 2: A high resolution TEM image showing an atomically sharp amorphous/crystal interface. [1] (a). TEM images of the cross-sectional morphologies of fully lithiated silicon nanowires (from left to right, the axial crystallographic orientations of the nanowires are $\langle 100 \rangle$, $\langle 110 \rangle$, $\langle 111 \rangle$, and $\langle 112 \rangle$). (b) Schematic of the amorphization process through the movement of amorphous-crystalline interface, occurring by the peel-off of the $\{111\}$ atomic facets.

intercalation of both c-Si and a-Si, the diffusivity of Si atoms within the Li_xSi phase is much lower than the Li atoms. When Li guest atoms diffuse into the host Si crystal and react, due to the lower diffusivity of Si atoms, a compressive stress is produced in the interface of Si and Li. Furthermore, the reaction between intercalated Li and intact c-Si lattice stimulate the host atoms to flow into the

old lithiated phase. When silicon reacts with lithium, the lithium atoms mostly concentrate on the c-Si/a- Li_xSi interface; however, new lithiated substructures also form inside the pre-lithiated layer by propagation of reaction-front to the remaining crystalline Si layers. The moving reaction front pushes previously lithiated layers out by the reactive flow and large deformation. Reactive flow in Silicon anode is assisted by lithium incorporation in breaking and reforming the Si-Si bonds. The stress distribution in the Si-NW during the lithiation process is obtained. The evolution of diffusion induced hydro-statics mean stress, $\sigma_m = (\sigma_{11} + \sigma_{22} + \sigma_{33})/3$ and von-Mises stress $\sigma^v = \sqrt{\frac{3}{2} s_{ij} s_{ij}}$, where $s_{ij} = \sigma_{ij} - \sigma_m \delta_{ij}$ is the ij component of deviatoric tensor, in Si-NW during the Li insertion. Compressive hydro-static stress hinders the lithium intercalation while tensile stress stimulates the Li atoms diffuse faster inside the Si-NW. The crystalline core experiences homogeneous hydrostatic compression, applied by the previously lithiated Li_xSi shell, which grows in magnitude when the core size decreases. This extra hydrostatics pressure retards the electrochemical reaction of Li with Si represented as



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Hybridizable Discontinuous Galerkin Finite Elements with Overset Meshing

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The finite element method is a solution technique used to numerically solve partial differential equations that may not have analytic solutions. There is an ever growing need to increase the accuracy of the solution, and reduce the computational cost associated with the numerical technique. These new solution techniques should address the following: parallelization, high-order accuracy, and accurate representation of the physical geometry regardless of the domains complexity.

First, a brief background on conventional (continuous Galerkin (CG)) finite elements. CG methods have been optimized to give accurate solutions to a variety of different engineering problems. With every solution technique there are always disadvantages. One of the main disadvantages with CG, especially from a fluid mechanics point of view, is that there is no local conservation between elements. To help correct this problem the Discontinuous Galerkin (DG) method was developed. DG methods mimic the finite volume approach because of local conservation [1]. Another advantage is that DG methods can handle irregular meshes that have hanging nodes [1], which is typically not the case when it comes to finite elements. Recently, DG methods have started growing in popularity, despite the fact that they have an increased number of degrees of freedom (DoFs) compared with CG.

To address computational cost the hybridizable discontinuous Galerkin (HDG) method is considered. HDG is a DG method that introduces a new primary variable, the numerical trace, into the weak formulation. The numerical trace approximates the global solution on the boundary of the elements from the local interior [2]. HDG shares the advantage with DG of ensuring local conservation by guaranteeing that the numerical trace is single valued. The DoFs associated with the numer-

ical trace are the only DoFs that are coupled globally, which considerably reduces the size of the global system. Since the local DoFs are decoupled HDG is highly parallelizable [3], which cuts down on computational costs. HDG also has advantages over DG such as increased stability, especially when using elliptic operators. Additionally, HDG is capable of exploiting cG techniques such as the Schur complement to statically condense the linear system.

Trying to increase the accuracy of the solution overset meshing is used to capture more complex geometric features of the domain. Overset meshing uses at least two different grids that overlap. Figure 1 shows a three dimensional shuttle that has been overlaid with overset meshes [5]. These meshes demonstrate how overset can be used to capture complex, and even three dimensional, geometrical structures. In order to take advantage of overset meshes, the boundary on a grid can have an arbitrary overlap region, or abut another grid. The communication between meshes occurs in the overlap region and brings rise to additional coupling terms in the weak formulation.

Coupling the high-order accuracy [1] of HDG with the ability to capture very complex geometries, like that shown in Figure 1, is the motivation for this research. This could be useful in fluid-structure interaction problems, for example, because one mesh could contain fluid information, while the other mesh could contain solid information but the two meshes could overlap at the fluid-structure interface.

Preliminary results for convection-diffusion and elastostatics problems are presented for the coupled HDG overset system. A comparison between non-overset HDG and the coupled HDG overset system will be discussed, but more analysis and numerical experiments need to be done to validate the coupling between the two techniques.

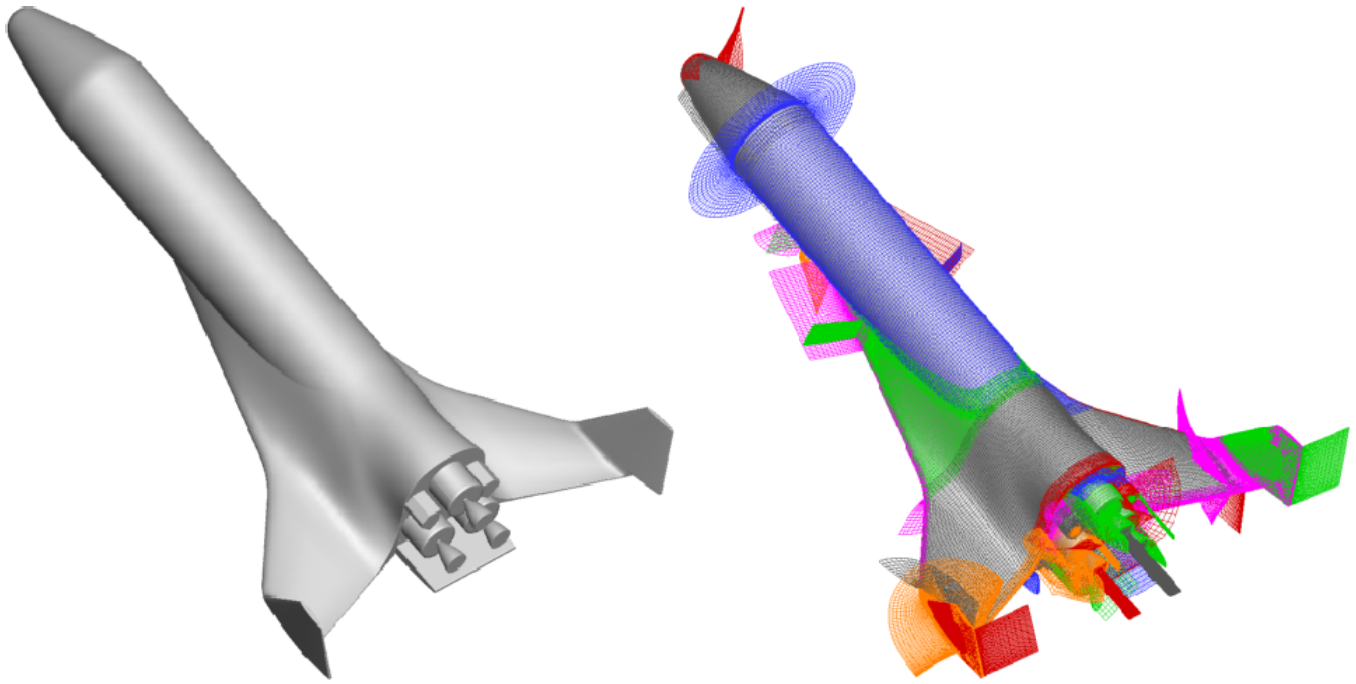


Figure 1: Full three dimensional space shuttle being represented with overset meshes from Galbraith et. al.[5].

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ULTRA-SMOOTH SHAPE MEMORY ALLOYS THIN FILMS PREPARED BY BIASED TARGET ION BEAM DEPOSITION

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NiTi based thin films have been primarily fabricated by vacuum magnetron sputtering as the common form of physical vapor deposition [1]. The films that exhibit shape memory behavior have found applications as micro-grippers, micropumps, stents, and endoscopes, among other micro-scale applications [2-4]. Reports on conventional NiTi thin films - used in practical application - recommend fabrication using vacuum magnetron sputtering utilizing a NiTi alloy targets. There are inherent drawbacks: Ni sputters at a rate nearly three times than Ti; Ti can be lost to residual oxygen; the target composition may not be absolutely uniform [1]. Essential to fabrication of NiTi thin films with the shape memory effect are controlling chemical composition, having uniformity of composition over a large area and run to run, and ensuring quality [1, 2]. To date, NiTi films exhibit shape memory behavior when thickness ranges from 0.5 to 2 μm [1]. Technological advancement for smaller scale applications requires the exploration of thinner films. In this work, NiTi alloy film with thicknesses on the order of 100 nm are co-sputtered from separate Ni and Ti targets utilizing biased target ion beam deposition (BTIBD) technique. BTIBD allows differential biasing of each target BTIBD and combines ion beam deposition and sputtering deposition, and offers low-pressure operation [5- 8]. A schematic of the BTIBD system is shown in Fig. 1. A low energy end-Hall (or closed-drift Hall) type ion source, typically lower than 25 eV, is introduced to the negative biased targets. A stable plasma must be maintained in the hollow cathode. The hollow cathode (HC) generates electrons and ejects electrons to the end-Hall ion source, rendering the plasma at the end-Hall constantly stable. A “wave” of ions carries the sputtered material to the substrate. Each target bias can be modulated differently by controlling the pulsed width and period. The capability of individual modulation can facilitate precisely controlling composition uniformity and stably maintaining deposition repeatability. Furthermore, bias target deposition allows control of medium energy Ar ions from the ion gun to impinge on the growing film and enables low ion energy bombardment with less impurities being sputtered. By design, on the other hand, the BTIBD technique enables controlling adatom energy (for high and low adatom energy process capabilities); decoupling

adatom energy and deposition rate as well as target and substrate plasma; and directing the flux while providing low energy ion bombardment at low processing pressures 1×10^{-4} to 5×10^{-3} Torr [8]. Thus, the technique is advantageous for the fabrication of ultra-thin and dense ultra-smooth films.

In this work, the BTIBD operating parameters are systematically adjusted for fine-tuning the alloy composition and deposition rate. We investigate very thin films (nearly 150 nm thick) compared to conventional shape memory NiTi thin films. We report findings of morphological observations in transmission electron microscopy (TEM), composition measurements in inductively coupled plasma atomic emission spectroscopy (ICP-AES), and surface roughness measurements from atomic force microscopy. The BTIBD films are compared to a control group of films deposited by the conventional magnetron sputtering in vacuum. Without optimizing the operating parameters, BTIBD yields high quality NiTi films of very thin dimensions.

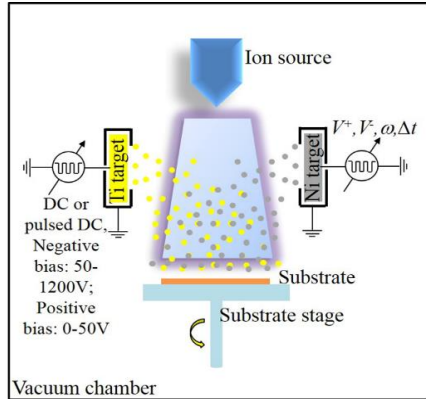


Figure 1: Illustration of co-sputtering system set-ups for the biased target ion beam deposition technique. BTIBD utilizes a high-ion-density, low-energy ion beam as a remote plasma source. Targets, orthogonal to the source and substrate, are then pulse-DC biased. The bias on target is to accelerate the low-energy ions for knocking out the target atoms. The sputtered target atoms are then depositing on the substrate to which the low energy ions can be directed. The broad-range, independent control on target bias and on ion beam source allow to control the adatom energies which in turn, tune the properties of the deposited film. The ultra-high processing pressure (up to 10^{-4} Torr) takes better care of oxygen contamination than sputtering ($>10^{-3}$ Torr).

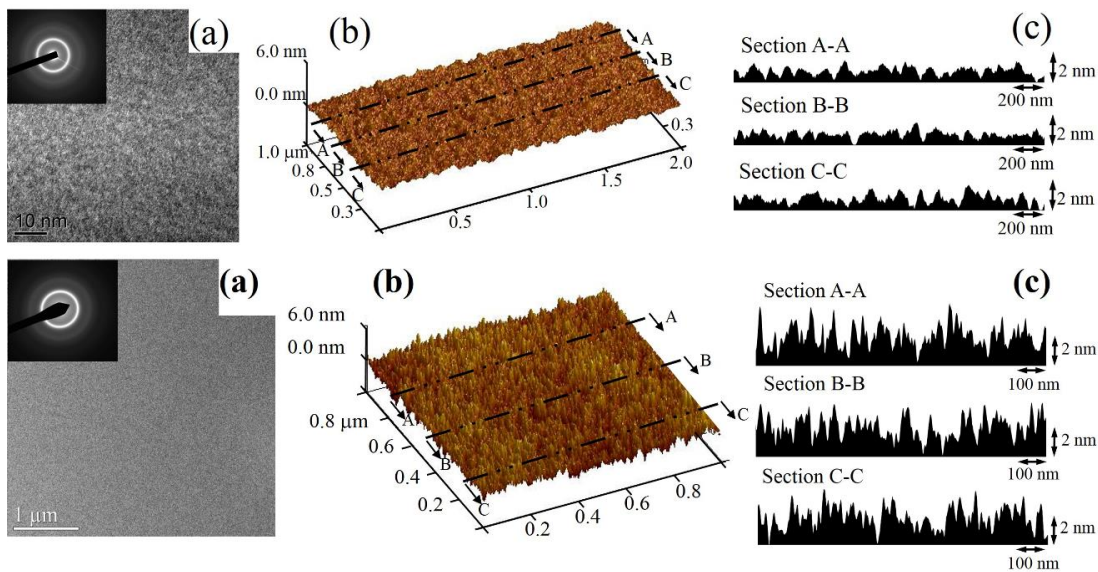


Figure 2: A BTIBD thin film [upper] versus magnetron sputtered thin film [lower] in the as-deposited state at room temperature: (a) TEM image with diffraction pattern illustrating that the film is amorphous; (b) Z-Max measurements from AFM analysis; and (c) cross-section profiles from (b)

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POSTER PRESENTATIONS

Towards a micromechanics based understanding of ultrasonic higher harmonic generation

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Nonlinear ultrasonics [1] has emerged as a powerful technology capable of early damage detection in structures. In this context, nonlinear ultrasonics refers to the generation of higher harmonic frequency components in the primary wave propagating in the material. Early investigations [2] identified two main factors that contribute to the above nonlinear effect:

1. elastic nonlinearity stemming from anharmonic potentials governing the motion of atoms in the solids.
2. dislocations.

This understanding spurred significant interest on the use of nonlinear ultrasonics for monitoring damage progression during fatigue [3] and creep [4] of structural metals. A simple 1D model is often employed to illustrate higher (second) harmonic generation. We start with the 1D version of the nonlinear stress-strain relation given by

$$\sigma = E\varepsilon(1 + \beta\varepsilon), \quad (1)$$

where ‘E’ is the Young’s modulus and ‘β’ is the nonlinearity parameter that quantifies micro-scale damage. The wave equation for the above material becomes

$$\rho \frac{\partial^2 u}{\partial t^2} = E \left(1 + \beta \frac{\partial u}{\partial x} \right) \frac{\partial^2 u}{\partial x^2}, \quad (2)$$

the solution for which can be written by a perturbation method as

$$u(x, t) = \frac{1}{8} \beta k^2 u_0^2 x + u_0 \cos(kx - \omega t) - \frac{1}{8} \beta k^2 u_0^2 x \sin(2kx - 2\omega t) \quad (3)$$

where ‘ω’ is the frequency of the wave, ‘k’ is the wavenumber and u_0 is the amplitude of the primary wave propagating in the material. As can be seen from Eqn (3), the amplitude of the second harmonic increases with the propagation distance and this increase is dependent on the ‘β’ parameter that quantifies micro-scale damage in the material. Thus, from a practical standpoint, the amplitude of the second harmonic can be used for monitoring damage progression in the material. However, this is not straight-forward when there are competing micro-scale mechanisms that affect the nonlinearity parameter in the material. Also, a simple 1D model as

the one presented above does not suffice for other scenarios of wave propagation such as during surface wave or guided wave propagation. To that end, we employ the following 3D constitutive model to depict the nonlinear material behavior.

$$W(E, \Gamma) = \frac{1}{2} \lambda(\Gamma) \text{tr}(E)^2 + \mu(\Gamma) \text{tr}(E^2) + \frac{1}{3} A(\Gamma) \text{tr}(E^3) + B(\Gamma) \text{tr}(E) \text{tr}(E^2) + \frac{1}{3} C(\Gamma) (\text{tr}(E))^3 \quad (4)$$

Here, $\lambda(\Gamma)$ and $\mu(\Gamma)$ are the Lamé’s constants that depend on the quantifiable aspects of microstructure denoted by Γ , and $A(\Gamma)$, $B(\Gamma)$ and $C(\Gamma)$ denote the higher order constants that depict nonlinearity in the material. It can be shown [5] that the Tension-Compression asymmetry in the material is responsible for second harmonic generation and we define an energy based measure ‘η’ that quantifies the asymmetry as follows

$$\eta = \frac{W(-E, \Gamma) - W(E, \Gamma)}{W(-E, \Gamma) + W(E, \Gamma)} \quad (5)$$

This work develops a micromechanics inspired homogenization based approach to predict the influence of microstructure on nonlinear material behavior and hence ultrasonic higher harmonic generation. This is based on the asymmetry measure (η) defined above. We illustrate this for the case of micro-voids in the material. We begin by considering a Representative Volume Element (RVE) that represents the microstructure of a statistically homogeneous material with micro-voids as illustrated in Figure 1. Each micro-void is assumed to be surrounded by a nonlinear material that represents localized plasticity as a driving force for voids to grow or coalesce. Here, we define the asymmetry parameter (α) for the RVE as the average as follows

$$\alpha = \frac{1}{V} \int \eta dV \quad (6)$$

Here ‘V’ is the volume of RVE. The above procedure is employed to quantify asymmetry and hence second harmonic generation. First, we compute the change in the linear elastic material parameters namely, Young’s modulus (E) and Shear modulus (G) as a function of volume-fraction of the micro-voids. Figure 2 shows that the linear elastic material

parameters change only by about 22% over a 10% change in void-fraction. On the other hand, Figure 3 shows the asymmetry as a function of the volume fraction for different sizes of nonlinear zone. Likewise, Figure 4 shows the normalized asymmetry where each of the curves in Figure 3 are normalized by their values at 1% void-fraction and all of them can be seen to coincide. Also, the change in the asymmetry is much larger ($\sim 1900\%$) when compared to the change in linear elastic material properties and hence nonlinear ultrasonics is much sensitive to micro-scale damage and this work develops a procedure to quantify nonlinear behavior due to micro-scale defects.

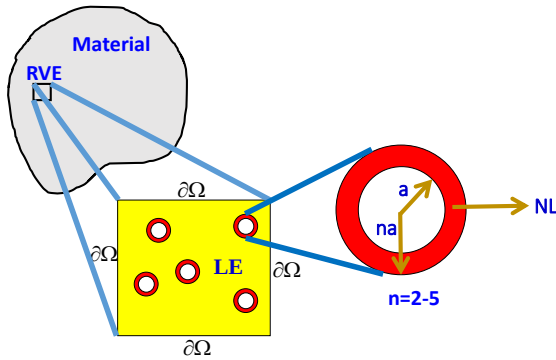


Figure 1: Schematic of RVE showing micro-voids

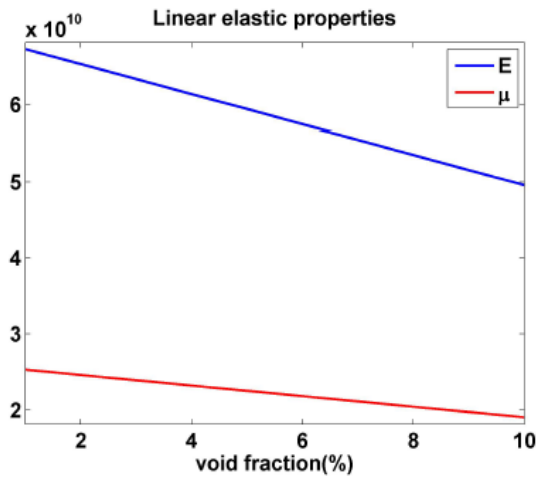


Figure 2: Linear elastic properties vs void-fraction (E- Youngs modulus, G- Shear modulus)

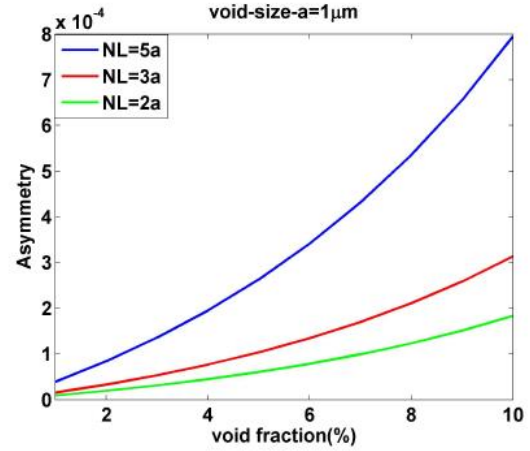


Figure 3: Tension compression-asymmetry vs void-fraction

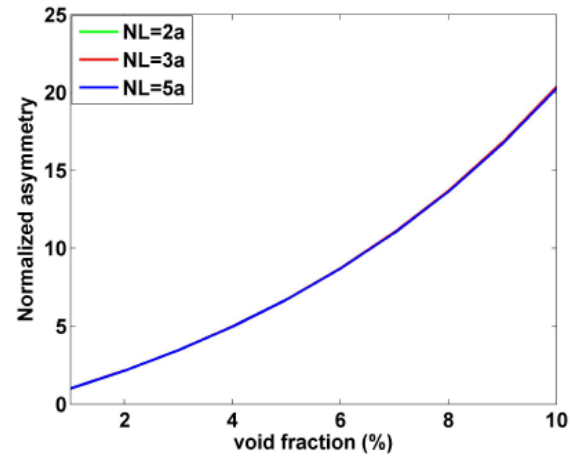


Figure 4: Normalized tension-compression asymmetry vs void-fraction

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ADHESION MECHANICS OF SQUID RING TEETH ELASTOMERIC PROTEINS

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Pressure-sensitive adhesive (PSA) can adhere to a variety of surfaces with pressure contact, and can be classified according to their physical state (e.g., aqueous, solvent and hot melt)^[1]. The chemistry of the adhesive formulation is based on the polymer type, molecular weight, level of cross-linking, and additives (e.g., tackifiers, fillers, stabilizers, and plasticizers). Commercial PSA's are generally obtained from petroleum based chemicals, such as acrylics, acetates, nitriles, and special (e.g., styrene based) block copolymers. Although natural elastomers are used as adhesives (e.g., natural rubber^[2], soy bean protein^[3]), to our knowledge, the number of reports related to bio-based PSA's is very limited. Additionally, natural PSA's typically have weak shear strength, and synthetic PSA's have cytotoxicity for medical uses.

There are other natural elastomers made from protein extracts, which have received significant interest as eco-friendly functional materials for underwater adhesion. Natural adhesives, such as

mussel, sandcastle worm glue and gecko feet, provide adhesion in wet or dry conditions. Mussel adhesion^[4] is based on a mixture of DOPA-containing proteins, which are able to provide various chemical-based surface interactions under wet conditions, including metal coordination^[5], hydrogen bonding^[6], and hydrophobic interactions^[7]. Gecko feet rely on Van der Waals interactions by exploiting the principles of friction and wetting at nanoscale for dry^[8] and wet^[9] adhesion respectively. However, the adhesion of these natural elastomers is different from the pressure sensitive adhesion mechanism, with a difference of up to two orders of magnitude in the adhesion strength.

Here, we studied the pressure-sensitive adhesive characteristics of a natural protein complex extracted from European common squid (*Loligo Vulgaris*). Squid ring teeth (SRT) is a thermoplastic hot melt PSA, which is plasticized by water above its glass transition temperature ($T_g = 32\text{ }^{\circ}\text{C}$). SRT does not require any drying process or toxic solvents, and

have good adhesion strength to a range of substrates at low temperatures. Due to its high tensile (~ 1.5 MPa) and shear strength (~ 2.5 MPa) in wet conditions and its natural biocompatibility, SRT provides unique opportunities of utilization as a hot melt adhesive. The bioelastomer adhesive could be used in an array of fields in the future, including dental resins, bandages for wound healing, and surgical sutures in the body, all of which require wet adhesion.

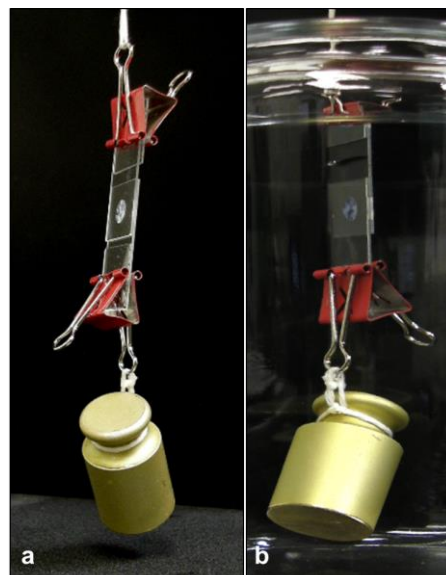


Figure 1: single-lap shear adhesion joints in dry (a) and underwater (b) conditions.

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Evaluating RF Sputtered SnS_x with *In Situ* and Post-Deposition Heating for Photovoltaic Applications

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During the most recent decades, one could argue that mankind has been relying on too heavily on fossil fuel for electrical and energy-use purposes. The world is continuing to grow as time passes, and the growing energy demands of the population are leading to an overconsumption of fossil fuels and a dramatic effect on our environment. One could also argue that as the cost of fossil fuels increases, items like gas and oil become only accessible to the upper and middle class, which will lead to more and more political and economic unrest. Scientists from all parts of the world are attempting to find the best solution for this exponentially increasing issue: a replacement for fossil fuel. This alternative fuel must be cheap and safe for the environment, yet with a high enough energy storage density to make it practical.

Numerous scientists have dedicated time and research to discover ways to produce energy other than with using fossil fuels, such as: wind farms, nuclear power, and hydraulic generators(1). Although a good start to alternative energy, none of these sources can produce efficient energy density per cost in comparison to gasoline. A source that is inexpensive but also environmentally friendly must be found. Currently, scientists from all parts in the world believe that photovoltaic cells can be a promising alternative fuel source.

Up to now, various types of solar cells have been suggested and developed: 1) inorganic solar cells incorporating inorganic semiconductor materials such as silicon and gallium arsenide (Si and GaAs), also next generation materials for thin film solar cells such as copper indium gallium sulfide (CIGS) and cadmium telluride (CdTe), 2) dye-sensitized solar cells (DSSCs) consisting of light-absorbing dye molecules, oxidized semiconductor material, redox electrolyte and catalyzed counter electrodes and 3) organic solar cells with light-absorbing polymer and conductive polymers (1). Solar cells with thin film absorber layers which have efficiencies of 20.4% and 20.8% have been produced using CdTe and CuIn_xGa_{1-x}Se₂ (CIGS), respectively (2).

Only two other universities in the United States (Harvard and MIT) have begun research on SnS trying to utilize its astonishing physical properties. SnS is a semiconductor material with a direct and indirect band gap of 1.33 to 1.55 eV and 1.07 to 1.39 eV respectively. It has an extraordinary absorption coefficient of $> 10^4 \text{ cm}^{-1}$ (3), and possesses the other ideal physical properties: cost efficient, non-toxic and

abundant in the crust of the Earth. Unfortunately, despite these excellent material properties, SnS has a low ionization potential of 4.7eV. A band misalignment is therefore needed. Previous studies carried by undergraduates Nicholas Tanen and Rafael Urena from my research group suggested that by using Mo and Ti top or bottom contacts and matching an heterostructure material, we will increase the efficiency of the device from 2% to above 10% in order to achieve the goal of cells that cost $< \$0.50/\text{Watt}$. According to the Shockley-Queisser limit, SnS and its bandgap can reduce the recombination mechanism that prevents a solar cell to convert sunlight into electricity effectively(4).

The objective of this thesis is to study SnS based solar cell devices, first by comparing the substrate configuration versus superstrate configuration and to calculate life time measurements for films made using an RF magnetron sputtering system with a SnS₂ target at different processing conditions. The deposition pressure, deposition times, and substrate temperature were studied in order to understand their effect on the SnS thin films. In order to understand their properties, the films are characterized morphologically, optically and electronically by field emission scanning electron microscope, X-ray diffraction, spectroscopic ellipsometry and transmission line method for film resistivity.

The first experiment of exploring different device configurations is comparing the substrate versus the superstrate configuration using SnS_x as an absorber, Ti as a metal contact, and ITO as the transparent conductive oxide (TCO). The two depositions runs performed were: one heated at 220°C and one at room temperature. One of the two ITO layer glass substrates experienced a replicate anneal treatment in temperatures as high as 500°C in order to replicate the heat treatment done in the first of the two depositions runs for this experiment

The second experiment involves a series of 9 depositions on CaF₂ glass substrates for transient absorption measurements (lifetime measurements). All depositions are done at 115W power, but different pressures (10, 42, 60 mtorr). The first 6 were made using in situ heating, and the 3 remaining were deposited at room temperature subsequently given a high temperature vacuum anneal(5).

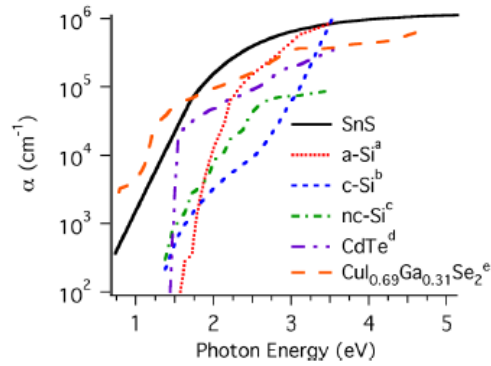


Figure 1: Absorption coefficient plot comparing conventional semiconductor materials achieving the highest efficiency percentage and SnS.

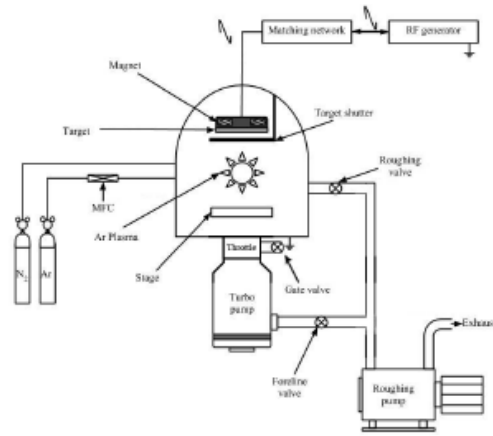


Figure 2: Schematic of the RF magnetron sputtering system.

1. Testing of Device Configuration

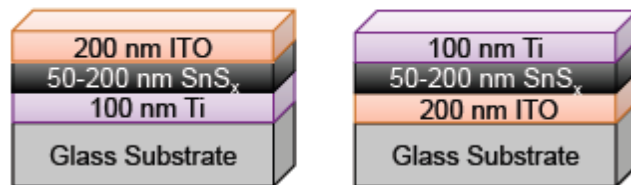


Figure 3: Substrate versus superstrate configuration (metal on bottom vs. metal on top).

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SILICA-COATED BaTiO₃/P(VDF-CTFE) NANOCOMPOSITES FOR ELECTRICAL ENERGY STORAGE

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In past decades, materials with high electrical energy storage have been paid considerable attention because of their promising applications in many fields, such as portable electronic devices, stationary power systems, and hybrid electrical vehicles. Among various energy storage devices, capacitors exhibit the advantage of high power density due to their fast electrical energy storage and discharge capability. In general, the energy density of dielectric materials for capacitors can be estimated by the equation, $U_e = \frac{1}{2} \epsilon_0 \epsilon_r E_b^2$, where ϵ_0 is the vacuum permittivity (8.855×10^{-12} F/m), ϵ_r is the relative permittivity, and E_b is the electric breakdown strength, respectively. According to the equation, the energy density of materials can be improved by increasing the permittivity or/and enhancing the breakdown strength.

Compared to other polymers, poly(vinylidene fluoride) (PVDF)-based ferroelectric materials have been widely studied as dielectric materials because of their large spontaneous polarization and high dielectric constants. The insertion of CTFE into the PVDF polymer chains can reduce the crystal size of the polymers, resulting in the reduction of remnant polarization and energy density loss. Another interesting approach to improve the energy storage properties of PVDF-based polymers is the addition of high dielectric constant particles into the polymers. The ceramic-polymer nanocomposites have attracted great attention because they can combine advantages from both dielectrics. Ceramic nanoparticles exhibit high dielectric permittivity, while polymer matrix can provide high breakdown strength, facile processability, low cost, and lightweight [1].

Although ferroelectric fillers obviously improve the dielectric constant of the nanocomposites, they also inevitably bring in an amount of free charge carriers and directly lead to the leakage current and conduction loss. The large contrast in permittivity between nanoparticles and polymer matrix can also generate highly inhomogeneous local electric field, resulting in a significant decrease in the effective breakdown strength [2]. Furthermore, the addition of nanoparticles that are not well-dispersed in the polymer matrix can give rise to the formations of particle aggregates and voids in the nanocomposites, causing the electronic conduction for high loss and dielectric failure at low fields [3].

In order to overcome these limitations, the surface modification of the nanoparticles has been

introduced. One of the most effective methods is the preparation of core-shell nanoparticles. Typically, the shell structures not only improve the compatibility between the fillers and the polymer matrix, but they also act as interparticle barriers to prevent a direct connection of ceramic particles. Due to their insulating properties, silica shells are supposed to play an important role in keeping the conductive network of nanoparticles in the composites to a minimum and then provide lower leakage current loss [4]. In addition, silica shells can be easily prepared onto the surface of nanoparticles and show a good compatibility with PVDF-based polymers.

In the present study, the nanocomposites of P(VDF-CTFE) with silica-coated BT nanoparticles have been prepared to investigate their dielectric properties and energy storage capabilities in comparisons to the pristine polymer and the nanocomposites with unmodified BT nanoparticles.

The core-shell BT@SiO₂ nanoparticles have been completely prepared by the sol-gel process of TEOS and characterized by fourier transform infrared spectroscopy (FTIR), dynamic light scattering (DLS), transmission electron microscopy (TEM), and zeta potential measurements. The well-dispersed and flexible nanocomposite films of P(VDF-CTFE) with BT@SiO₂ nanoparticles have been fabricated by solution casting, and then hot pressing process. According to DSC experiments, there are no significant changes in thermal properties and crystal structures of BT@SiO₂/P(VDF-CTFE) nanocomposites, compared to the pristine polymer and the BT/P(VDF-CTFE) nanocomposites. It can be concluded that dielectric properties and energy storage capabilities for the nanocomposites are not relevant to the changes in their crystal structure. Compared to the pristine polymer, BT/P(VDF-CTFE) and BT@SiO₂/P(VDF-CTFE) nanocomposites obviously exhibit greater dielectric permittivity due to the addition of nanoparticles with high dielectric permittivity. However, a decrease in electrical breakdown strength and higher energy loss are observed in the BT/P(VDF-CTFE) nanocomposites owing to a presence of additional conduction pathways, an aggregation of BT nanoparticles, and large differences in local electric field in the materials. Apparently, these drawbacks can be reduced by the surface modification of BT nanoparticles by silica coating. In comparisons to the pristine polymer and the nanocomposites with

unmodified BT nanoparticles, the BT@SiO₂/P(VDF-CTFE) nanocomposites provide higher dielectric permittivity and lower energy loss (Figure 1). The BT@SiO₂/P(VDF-CTFE) nanocomposites also exhibit higher electrical breakdown strength due to the increases in electrical resistivity and mechanical strength (Figure 2). Moreover, the BT@SiO₂/P(VDF-CTFE) nanocomposites possess the highest charge-discharge efficiency, compared to the pristine polymer and the BT/P(VDF-CTFE) nanocomposites (Figure 3). These superior properties are mostly attributed to the insulating silica shells on BT@SiO₂ nanoparticles. They can enhance the electrical resistivity and mechanical strength in the nanocomposites and reduce the local electric field differences between particles and polymer matrix. In addition, the silica shells of BT@SiO₂ nanoparticles can lead to better interfacial interaction between two phases, producing more homogeneous quality films. These results strongly suggest a great potential for the nanocomposites of ferroelectric polymer with silica-coated high permittivity nanoparticles in energy storage applications.

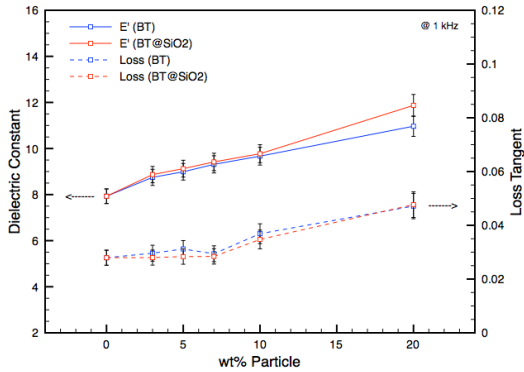


Figure 1: Dielectric permittivity and loss tangent of pristine P(VDF-CTFE), BT/P(VDF-CTFE) nanocomposites, and BT@SiO₂/P(VDF-CTFE) nanocomposites at 1 kHz and room temperature.

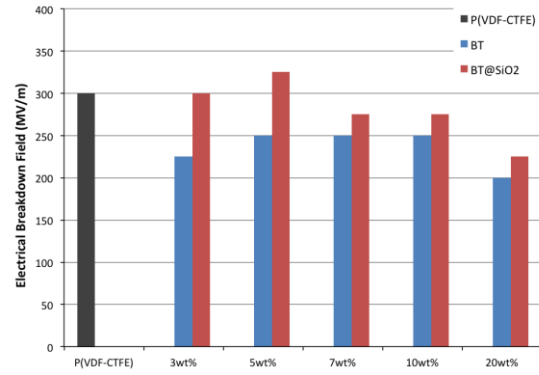


Figure 2: Breakdown electric field of pristine P(VDF-CTFE), BT/P(VDF-CTFE) nanocomposites, and BT@SiO₂/P(VDF-CTFE) nanocomposites.

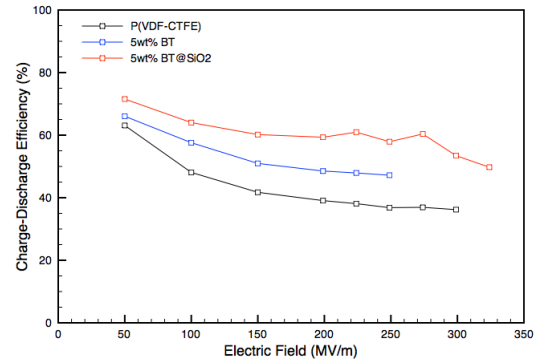


Figure 3: Charge-discharge efficiency of pristine P(VDF-CTFE), 5wt% BT/P(VDF-CTFE) nanocomposite, and 5wt% BT@SiO₂/P(VDF-CTFE) nanocomposite as a function of the applied electric field.

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DIELECTRIC PROPERTIES OF COLUMNAR AND BULK PARYLENE C FILMS IN THE INFRARED REGIME

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While it is known that the deposition process of inorganic thin films affects its physical properties, not much information is available in the literature about organic thin and microfibrillar films. Recently thin films of Parylene C [1], a polymeric material, have been explored for variety of biological and engineering functions in both homogeneous and inhomogeneous forms. The cross-sectional morphology of the inhomogeneous films can be engineered to comprise microfibers of columnar, chevron and chiral shapes [2]. Films comprising columns of microfibers called columnar thin films (CTF). In exploring different physical properties and applications for these inhomogeneous Parylene C films we found that the CTFs of Parylene C have more number of crystal planes and smaller crystal sizes than a traditionally deposited bulk film, as shown in Fig. 1. Thus, the physical properties of CTFs are expected to be different than a bulk film. Our interest lies in exploring the inhomogeneous thin films (including CTFs) as photonic crystals. With the knowledge of experimentally feasible dimensions of CTFs microfibers, band gaps are expected in the mid and far-infrared regime. Here, we report the dielectric properties of the CTF and bulk film in the infrared regime of electromagnetic spectrum in terms of the Lorentz-Drude model parameters.

Silicon and brass substrates of dimensions 0.5×0.5 in² are cleaned with standard cleaning procedure SC-1, prior to deposition. The CTF is fabricated by focusing the Parylene-C monomer vapor normally onto the substrates. In addition to the CTF, a bulk film is fabricated in the reduced capacity chamber using identical amount of dimer (4 gms). The deposition parameters of furnace 690°C, vaporizer 175 °C, and vacuum 28 mTorr were the same for both kinds of depositions. The cross-sections of CTF imaged by a scanning electron microscope revealed parallel strands of microfibers of diameter 5 μ m and placed 1-2 μ m apart. The CTF

and bulk film were found to be 165 μ m and 8.8 μ m in thickness.

Attenuated Total Reflectance (ATR) spectroscopy experiments in the frequencies between 12 and 120 THz was performed on the CTF using a Bruker Vertex V70, Fourier Transform Infrared (FTIR) spectrometer. The CTF and a Zinc-Selenide (ZnSe) crystal are held in the kretschmann configuration. Experiments were performed using S- and P-polarization light at an incidence angle of 45°. The bulk film is peeled off the silicon substrate using a razor. Transmission spectroscopy in the same frequency range is performed using a Bruker Hyperion 3000 FTIR microscope. Unpolarized light was used for the transmission mode of experiment.

The calculated reflectance for the CTF in ATR mode is shown in Fig. 2. We note from Fig. 2, a large number of optical resonances are present for the CTF. A similar phenomenon is also observed for the bulk film. Hence, the relative permeability is considered as the sum of Lorentz-Drude models and analytical functions are formulated to determine Reflectance in both ATR and Transmission experiments. The usual non-linear least squares regression failed to validate a test case (with large number of resonances) in inversely determining the optical (or dielectric) properties. Hence, these properties of CTF and bulk Parylene-C films are determined using hybrid scheme optimization via Genetic Algorithm in Matlab. Prior to this, the algorithm is validated with the case of deionized water over ZnSe.

The dielectric properties of CTF and bulk film are determined in terms of Lorentz-Drude model (LDM) parameters. These frequency dependent dielectric properties help in determining the electromagnetic wave dispersion characteristics. This work also highlights the change in optical properties due to modified deposition process.

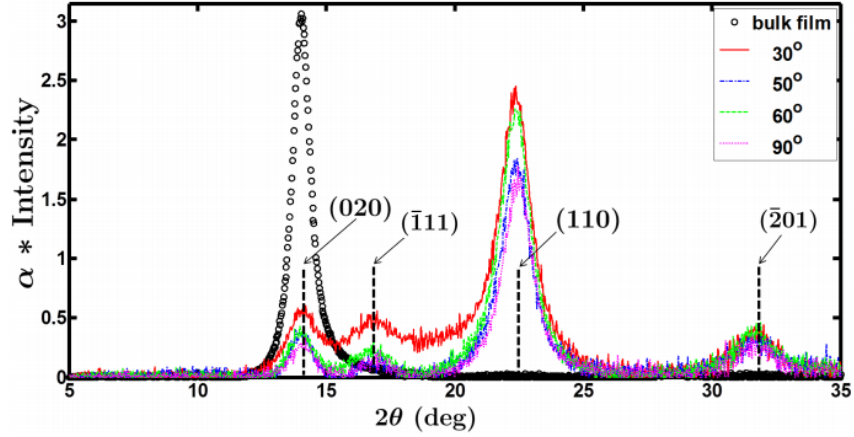


Figure 1: Comparison of XRD patterns of four different columnar thin films ($\chi_v \in \{30^\circ, 50^\circ, 60^\circ, 90^\circ\}$) and the bulk film. The normalization factor $\alpha = 5 \times 10^{-4}$ for all μ FTFS but $\alpha = 10^{-4}$ for the bulk film. The Miller indices for the crystal plane for each peak are also provided.

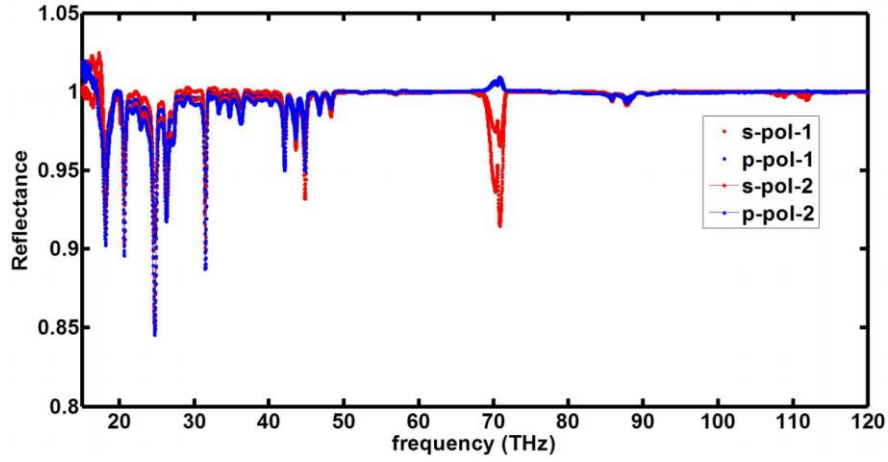


Figure 1: Experimentally measured reflectance of S- and P-polarization of two columnar thin films via Attenuated Total Reflectance spectroscopy.

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Spreading depression is a wave-like neural phenomenon that occurs in the cortex of the human brain and is linked to disorders of the brain such as migraine, epilepsy, and stroke. We propose a cellular model of the brain that, with only differences in initial conditions, replicates the cellular dynamics of these pathological phenomena. This ability to unify these oft-thought disparate phenomena lies in a few important changes to standard neural modeling. For these pathological states, large deviations in the ionic concentrations and energy use in the cellular environment, properties typically ignored in computational neural models, is a critical feature that must be represented. Building and investigating a model of spreading depression that tracks these variations allows us to determine best practice for understanding and treating or preventing the disorders it is associated with in real brain tissue.

Leao in 1944 first discovered spreading depression behavior in an experiment on the nature of epilepsy in rabbits [1]. After inducing seizures in the animals, there would be episodes of silence in the EEG that slowly but progressively spread across the recording sites. Both the depression of activity and its progressive spread within the brain lead to the description as spreading depression (SD) or cortical spreading depression. Since Leao's experiments, SD has undergone many experimental and theoretical studies in cellular, tissue, and whole animal models, and yet many questions still remain as to how the phenomenon is initiated and how it spreads.

The model we propose builds upon the cellular model of Hodgkin-Huxley, with a set of partial differential equations where the dynamics of the cellular environment are modeled as an electrical circuit [2]. The local potential difference across a cell membrane is altered by the flux of ions across the membrane and the conductance of the membrane as determined by Ohm's law.

In SD, large changes in ion concentration can occur compared to the

expected changes in the micro-environment of functioning neural cells [3]. An important addition made to this model is thus to track the changes in ionic species that occur in addition to the electrical behavior. Additionally, the movement of these large charged particles will create osmotic pressure differences that alter the movement of water within the cellular environment, and hence change intra- and extra-cellular volumes, which further affects the changes to ionic concentration. Additionally, in extreme circumstances of ion change, the cell will use many active mechanisms to re-establish cell equilibrium, a process that requires higher than usual amounts of energy. We monitor the activity of energy usage by the cell in the local environment, as a key variable for the ability of the cell to function as well as measure its overall health.

The model as described above is simulated through numerical integration with experimentally determined parameters. With appropriate changes to a few key parameters that affect the energy available to the cell, as well as the ionic environment of the cell, we replicate the behavior of SD, as well as seizure and stroke.

With this generalizable model, we demonstrate the plausibility and effectiveness of control schemes to alter the neural dynamics so as to prevent or modulate the pathological phenomenon of not only SD but related behaviors of seizure and stroke as well. We demonstrate the efficacy of three control schemes, with increasing complexity: proportional control, variance based bifurcation control, and Kalman-filter control.

The implemented controllers provide novel approaches for universal treatment of neural tissue, to maintain a stable environment that avoids excessive demands on energy, as well as significant disruptions to the local ionic environment. This model-based control lays a foundation for medical technology that monitors critical features of brain dynamics and supplies an appropriate and safe treatment stimulus.

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FEASIBILITY OF USING LASER-SUSTAINED PLASMA FOR NITRIDING OF COMMERCIAL PURE TITANIUM

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Titanium and its alloys have been studied widely over the past few decades because of several interesting properties, such as: 60% lower density than steel or nickel-base superalloys, comparable tensile strength to steel, good corrosion resistance, and biocompatibility. However, the mechanical application of titanium has been limited by its poor tribological properties, especially its low wear resistance and high friction coefficient with itself and other metals. Laser nitriding is a promising method of improving the tribological properties of titanium. In this method, the titanium substrate is scanned under a focused laser beam in the presence of nitrogen gas flow. Due to the high power input to the surface, it melts, forming a molten pool at least as wide as the laser spot size. Nitrogen readily diffuses into liquid titanium, and is further transported deeper in the melt pool by convection. Upon solidification, TiN_x and $\alpha\text{-Ti (N)}$ are formed, where x depends upon the concentration of nitrogen transported in the melt pool. The main advantages of laser-assisted nitriding methods over other nitriding methods (such as chemical or physical vapor deposition) are less processing time and a strong metallurgical bond between the surface layer and the substrate; however this method is subject to cracking due to thermal stresses.

Laser-nitriding has been widely studied and reported in literature for the past 30 years; however, the role of near-surface plasma has not been well understood. Nassar *et al.* investigated the role of near-surface plasma in the open-air nitriding of titanium using lasers-sustained plasma [1]. Laser-sustained plasma (LSP) is plasma that can be struck and sustained indefinitely near the focus of a high-powered CO_2 laser without enclosures or oxygen shielding devices (figure 1). They studied: (1) conditions where titanium can be nitrided using pre-struck nitrogen LSP scanning the substrate; (2) comparable conditions where nitriding with a laser beam occurs without plasma; and (3) conditions where nitriding occurs with surface-struck plasma. Nassar *et al.* discovered a new processing regime where nitriding can be conducted in an open atmosphere using pre-struck LSP. LSP was found to shield the substrate from oxygen contamination, and also to efficiently transfer power to the substrate generating a melt pool of similar size to that formed with the laser beam alone. The larger OFD of the pre-struck LSP permitted wider surface coverage and

thus faster nitriding at the same scanning speed than possible with the surface struck plasma.

This research advances the work of Nassar *et al.* by studying microstructures as a function of processing parameters during LSP nitriding of commercially pure titanium (CP-Ti) in open atmosphere. The main process variables are laser power, off-focal distance, gas flow rate, nitrogen:argon ratio, and specimen scan speed. In this work, we deposited single nitride trails by varying scan speed, off-focal distance (and hence spot size) and nitrogen-argon ratio. Surface morphology, transverse cross sections, and crack formation were studied by utilizing optical and scanning electron microscopy. Weight measurements of the nitrided CP-Ti substrate were performed to study the nitrogen intake into the melt pool as a function of argon dilution. Optimal conditions were identified from single nitrided trail data which will be used to deposit multiple overlapping nitride trails in future work.

Figure 2 shows the effect of nitrogen dilution (by argon) on surface and cross-section microstructure. The addition of argon to the nitrogen gas flow in the plasma had a significant effect in decreasing nitrogen intake into the melt pool. Decreasing the nitrogen concentration by 11 % caused the nitrogen intake to decrease by 60 % and significantly reduced crack formation on the surface. Surface dendrites of TiN were observed to increase with decreasing speed and decreasing $\text{N}_2:\text{Ar}$ ratio. Argon addition reduces the surface roughness by reducing surface tension gradients on the surface of the melt pool. Marangoni convective effects are seen to diminish at $\text{N}_2:\text{Ar}$ ratios of 16:2 and below. This prevents the sub-surface Ti-rich liquid to be exposed to the nitrogen atmosphere, hence limiting the nitrogen intake to diffusion rather than a combination of convection and diffusion.

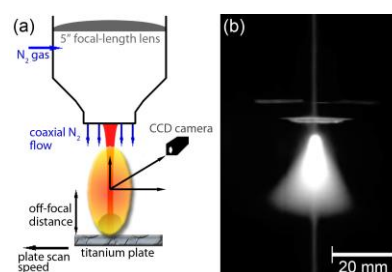


Figure 1: LSP nitriding: a) Schematic b) CCD image

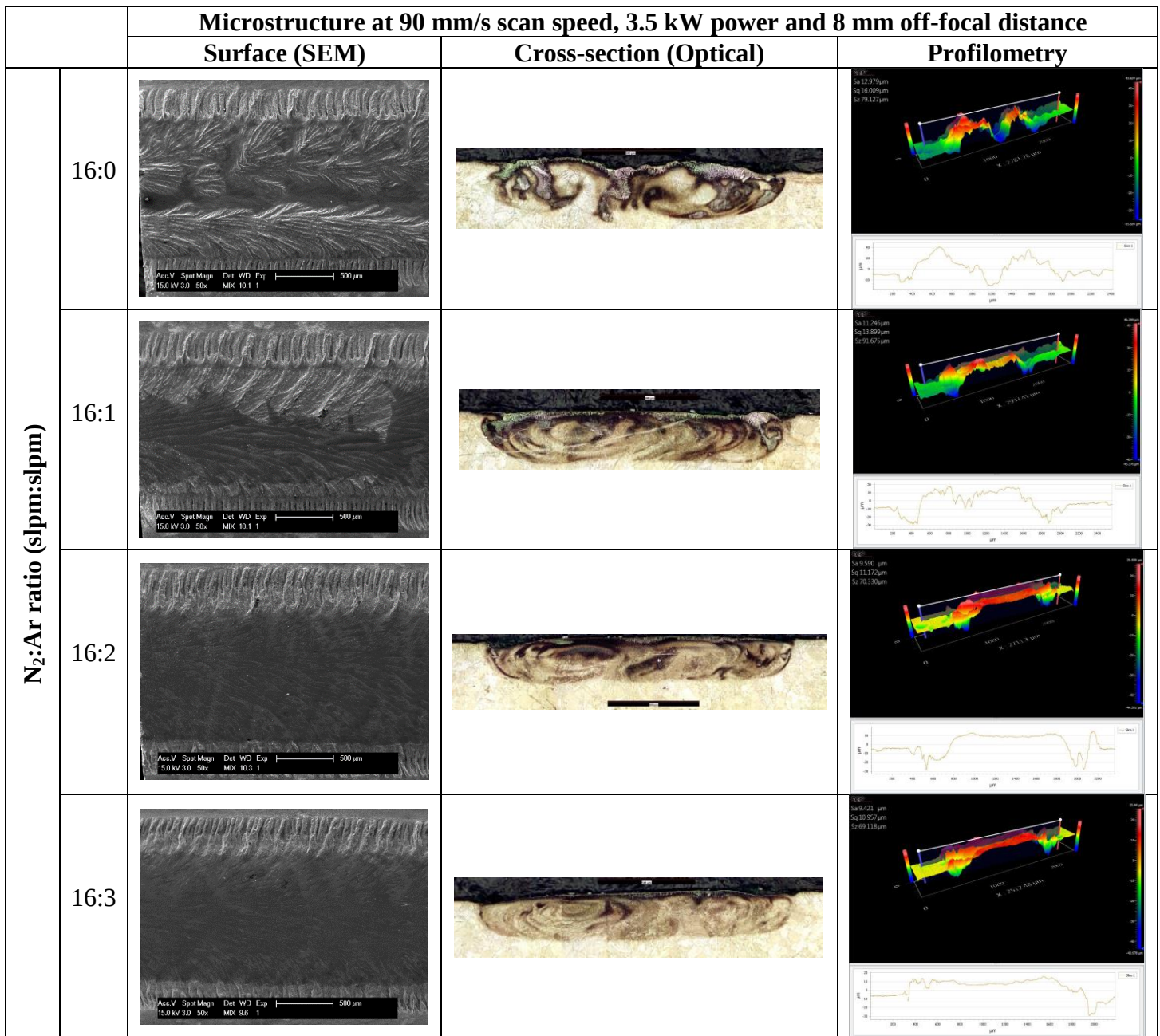


Figure 2: SE micrographs and optical profilometry data of surface topology, and optical micrographs of cross-section as a function of nitrogen dilution. Addition of argon decreases surface roughness and limits the nitrogen intake mechanism into the melt pool to diffusion rather than convection-diffusion.

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Development of All-Dielectric Plasma Metamaterials

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The first theoretical investigation into “left-handed” materials with simultaneously negative values of permittivity and permeability was carried out by Veselago in 1964. Several interesting effects were predicted for left-handed materials including a reversed Doppler effect and a negative index of refraction [1]. Natural materials are not left-handed, but structures - often containing sub-wavelength elements - have been fabricated which can exhibit the exotic properties predicted by Veselago; such structures have been coined “metamaterials”. Metamaterials have gained much attention after publications suggesting the possibility of creating superlenses and invisibility cloaks [2,3]. Both the superlens and the invisibility cloak were demonstrated experimentally within a few years of the theoretical publications [4, 5]. More generally, metamaterials are promising for their ability to offer control over electromagnetic radiation.

In the past decade, the concept of plasma photonic crystals was introduced and experimentally verified [6]. More recently, it was shown that plasma arrays suitable for use as photonic crystals or metamaterials could be generated using split ring resonators under microwave irradiation [7]. One may describe this as a metamaterial produced by another metamaterial. Such metamaterials based on plasmas are promising since they are tunable in terms of permittivity and the elastic collision frequency of electrons, which means, for instance, that they can act as reflectors or absorbers; they also operate in a wide frequency range from GHz to THz. Quick changes to the plasma can occur through increasing microwave power and gas pressure experienced by the plasma. It is also interesting to note that plasmas intrinsically have a negative permittivity. Furthermore, plasmas can be mixed with other structures such as metal rings or have internal structure to allow for even more functionality [6].

While many metamaterials rely on metal structures such as rings and rods, it has also been demonstrated that metamaterials could be made completely of dielectric materials [8]. Dielectric materials also may be valuable for use in generating plasma metamaterials. The split-ring resonators used to generate plasmas mentioned earlier suffer due to poor energy utilization. Dielectric resonators may offer substantial (orders of magnitude) increases in the quality factor (Q), the ratio of energy stored to energy lost in a resonant structure.

There are many challenges associated with creating all-dielectric, plasma metamaterials. First, the electrical properties of the materials must be understood at varying temperatures, which they may encounter when subjected to plasma. Non-thermal (“cold”) plasmas will most likely be used, and cold plasma temperatures can range from room temperature to 2500 Kelvin. In addition to finding/fabricating materials that have desirable behavior under varying temperature conditions, it is also important to concentrate electromagnetic energy in order to ignite and sustain a plasma. The following describes initial investigations into electrical properties under varying thermal conditions and into concentrating electromagnetic energy.

A wide variety of dielectric materials are chosen as a starting point for testing. Ferro, Heraeus, Dupont 943, Dupont 951, alumina, quartz, and rutile are subjected to temperatures in the range 50-600°C as well as frequencies from 100Hz to 1MHz. The permittivity ϵ_r and loss tangent $\tan\delta$ are studied under the previously described experimental conditions. In addition, the permittivity and loss at high frequencies (GHz) are studied using the split-cavity technique. High-frequency and high-temperature results are tabulated in Table 1. Lower loss tangents are desirable whereas the permittivity range offers flexibility in design of future devices. At high temperatures alumina, Heraeus, and Ferro look most promising.

In order to concentrate electromagnetic waves, waveguide modes are studied in cylindrical dielectric resonators. As a first foray into the possibilities, the transverse electric field mode (TE₀₁₁) is considered. A dielectric resonator composed of $\text{Zn}_{0.8}\text{Sn}_{0.2}\text{TiO}_4$ is halved so that the electric field amplitude in the gap is increased and plasma may be formed in the gap. The halved resonator is shown in a Hakki-Coleman setup as shown in the inset of Figure 1. The shift in the resonant frequency of the mode in the Hakki-Coleman setup is studied as a function of distance as seen in Figure 1. The change in the slope of the graph at a gap distance of 0.31mm suggests other modes other than the TE₀₁₁ mode are being excited or that the two halves of the resonator may be resonating independently and coupling to each other. As expected from electromagnetic boundary conditions, simulation results (not shown here) give evidence that the electric field enhancement in the gap is proportional to the permittivity of the material.

Table 1: Tabulated below are the relative permittivity ϵ_r and loss tangent $\tan\delta$ of various dielectric materials under two conditions: high-frequency ($>4.4\text{GHz}$) and room temperature (21°C) and low frequency (1MHz) and high temperature (600°C).

Material	ϵ_r at 600°C & 1MHz	ϵ_r at 21°C & greater than 4.4GHz	$\tan\delta$ at 600°C & 1MHz	$\tan\delta$ at 21°C & greater than 4.4GHz
Ferro	11.6	5.883	.15	.0012
Heraeus	13.7	8.436	.083	.0037
Dupont 943	41.5	7.281	1.5	.0013
Dupont 951	20.3	7.376	.58	.0069
Quartz	7.20	3.763	.33	.00036
Alumina	14.0	9.065	.056	.00077
Rutile	119	100.3	.71	.00042

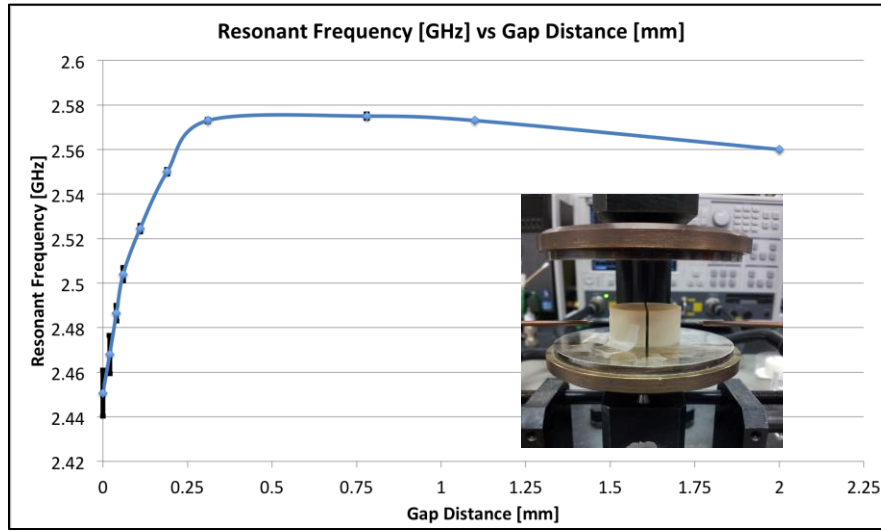


Figure 1: Resonant frequency of the TE_{011} mode is shown as a function of the gap distance between the two halves of the resonator. In the inset, a Hakki-Coleman setup for studying dielectric properties is shown. In the center, the halved resonator is visible with two silver-coated plates above and below it. The plates set up conductive boundaries at the ends of the cylinder upon contact. The probe on the left is used to excite electromagnetic modes in the resonator and the probe on the right is used to collect the resonator's response to excitation.

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STRUCTURE AND INTERFACE OF NANOSCALE TiNi THIN FILM PREPARED BY BIASED TARGET ION BEAM DEPOSITION

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To date, sputtering is the most widely used method for deposition of TiNi shape memory alloys thin films. [1-3] The underlying mechanism of shape memory actuation is martensitic phase transformation, in the case of TiNi, between B2 crystal structure (parent phase) and B19' crystal structure (product phase). [4] The limit on the minimum thickness of sputtered TiNi film is reported to be associated with resistance forces from diffusion at the substrate/film interface and surface oxidation. [2] The resistance forces can prevent the lattice distortion and twinning involved in the transformation, thereby inhibiting the self-accommodation morphology. Diffusion at the substrate/film interface results from heat-treatment which is the typical means to crystallize the as-deposited amorphous TiNi films. [5, 6] After heat-treatment, the interfacial diffusion layer is 120 nm in TiNi film with 4 micron thickness[7], and is 10 nm in 234 nm film[8]. As film thickness decreases further, the diffusion layer thickness could account for over 15% of the film thickness; such ratio is imposing pronounced constraint, and even suppress on MT. [5, 8] On the other hand, the issue of oxygen contamination can be avoided through using high vacuum because less residual oxygen is present in high vacuum, thereby less chance to react with titanium atoms.[6] Advantageous synthesis method is expected to provide solution to minimize the ratio of diffusional layer thickness to film thickness and meanwhile to produce parent phase in order for thinner TiNi film to exhibits MT.

Biased target ion beam deposition (BTIBD) technique, a recently-developed synthesis method able to produce high-quality films [9-11], is employed. The current authors have recently demonstrated the potential of BTIBD to synthesize TiNi thin films with precise control of composition (down to 0.5 atomic percent), broad composition range (from 28 to 74.6 at %), smooth surfaces (less than 0.3 nm roughness), and crystallographic structure of B2 and B19' for thin films with 100 nm thickness. [12] BTIBD utilizes a high-ion-density, low-energy ion beam as a remote plasma source. Targets, orthogonal to the source and substrate, are then pulse-DC biased. The bias on target is to accelerate the low-energy ions for knocking out the target atoms. The sputtered target atoms are then depositing on the substrate to which the low energy

ions can be directed. The broad-range, independent control on target bias and on ion beam source allow to control the adatom energies which in turn, tune the properties of the deposited film. The ultra-high processing pressure (up to 10^{-4} Torr) takes better care of oxygen contamination than sputtering ($>10^{-3}$ Torr) [9]. Details of this technique have been reported in our previous work [12] and elsewhere [13, 14]. BTIBD has also been demonstrated to produce films with highly uniform thickness (within 3% across 4 inch wafer) [15], less "overspill" contamination [16, 17], and less interlayer mixing (in multi-layer) [17, 18].

The minimum thickness of sputtered TiNi film to exhibit apparent MT is 100 nm. [5, 6] With decreasing thickness, the resistance forces become severe so that MT is suppressed below a critical film thickness. [5, 8, 19, 20] It is the goal of this report to assess the ratio of diffusional layer thickness to film thickness, and the existence of the essential B2 structure within sub-100-nm BTIBD film.

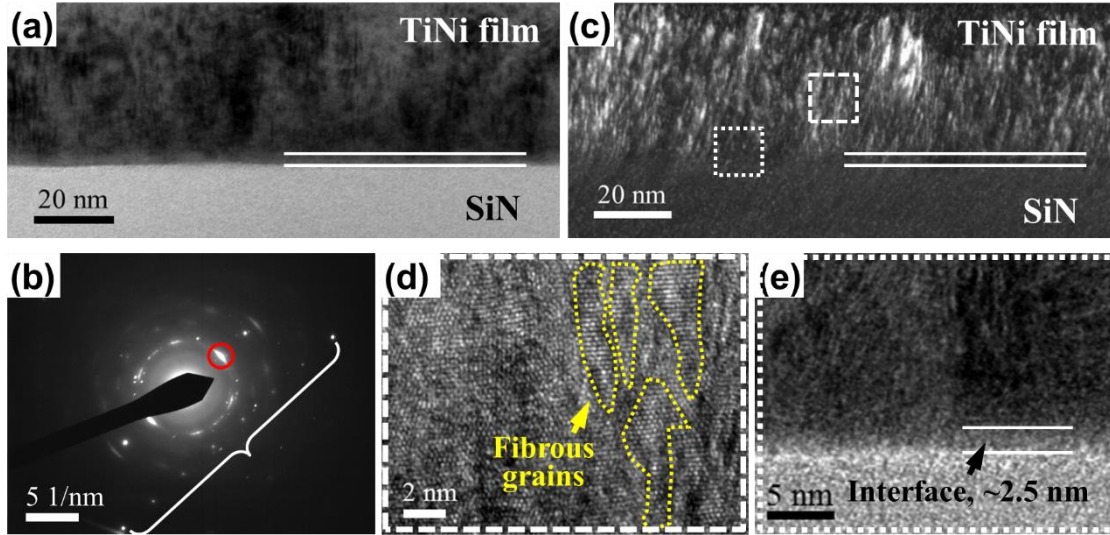


Figure 1: TEM bright-field a) and dark-field micrographs c), diffraction pattern b), High Resolution TEM image d) and e) of the cross-section in TiNi film. In a) and c), the two white lines delineating the interface between TiNi film and SiN substrate are the same as the ones in d). The white bracket in b) highlight the directionality of diffraction spots. c) is corresponding to the red-circled diffraction spot in b). d) and e) are zoom-up images of the regions within the dash-white-dot box and square-white-dot box in c). The yellow lines in d) are depicting some of the grains.

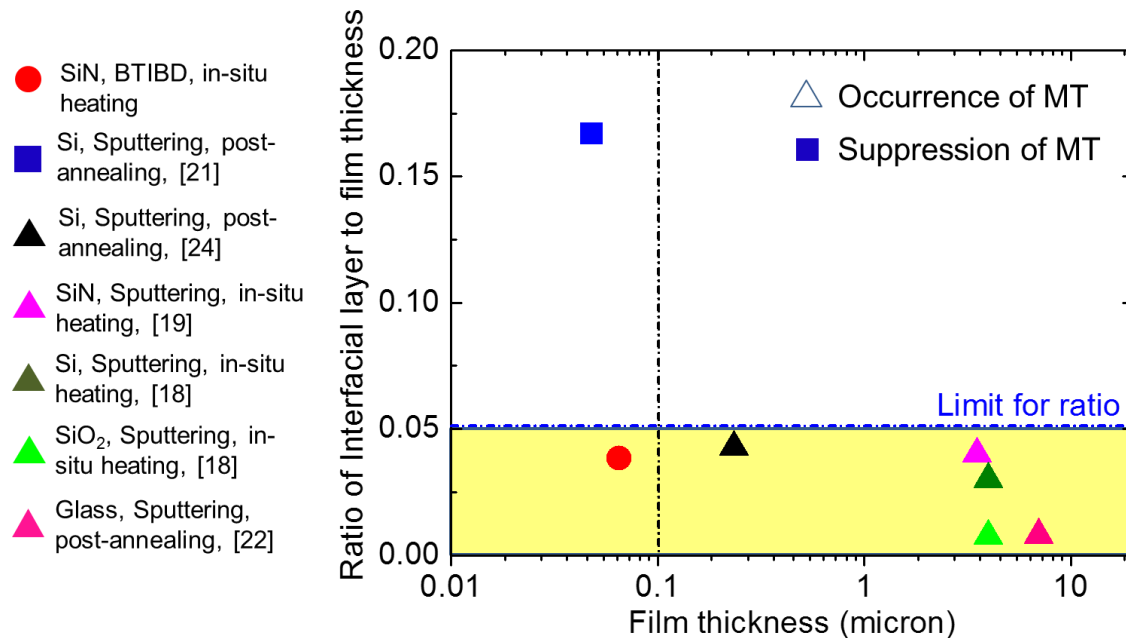


Figure 2: Plot of diffusion layer thickness to film thickness ratio versus film thickness. The references for square and triangle data point, and the fabrication conditions are listed beside the plot. The red data point is from the current study.

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